DATA-DRIVEN MAINTENANCE

PLANNING, SCHEDULING, AND CONTROL

A Dissertation

by

CHRISTOPHER AMPOFO KWADWO GORDON

Submitted to the Office of Graduate and Professional Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

Chair of Committee,	Efstratios N. Pistikopoulos
Committee Members,	Mahmoud El-Halwagi
	Joseph Sang-Il Kwon
	Sergiy Butenko
Head of Department,	Arul Jayaraman

May 2021

Major Subject: Chemical Engineering

ABSTRACT

Maintenance refers to acts undertaken to improve the availability and integrity of ageing productive systems, and is at the nexus of the broader concepts of system resilience and system effectiveness. Compromised system resilience can reduce system effectiveness and can lead to catastrophic consequences such as cost to human life due to process safety incidents, lost revenue due to downtime, as well as damage to the system and the environment. Data analytics and mathematical optimization are key research areas that are well positioned to offer solutions that leverage increasing data proliferation and help address the complexities associated with process-maintenance interactions. The present work optimizes maintenance at multiple time-scales using both data-driven and first-principles methods while simultaneously optimizing production. The work is divided into three major areas: (1) maintenance planning, which explores the effects of imperfect maintenance and uncertainty in model parameters; (2) data-driven prescriptive maintenance, which involves future failure prediction via machine learning and optimal process and maintenance scheduling; and (3) maintenance-aware predictive control, which lies at the interface of predictive maintenance and multi-parametric model predictive control. This work makes advances in process safety engineering and process systems engineering while also developing advanced, systematic and mathematical tools for decision support.

DEDICATION

To loved ones, both present and departed.

ACKNOWLEDGEMENTS

Special thanks are expressed to the late great Professor Christodoulos A. Floudas for his vision and encouragement.

This research would not have materialized without the insightful guidance of Professor Efstratios N. Pistikopoulos and the late Professor M. Sam Mannan. It was an honor to learn from their immense wisdom.

Professors Mahmoud El-Halwagi, Joseph Sang-Il Kwon, and Sergiy Butenko were a pleasure to interact with and helped provide a sense of comfort.

Highly enjoyable discussions with Dr. Melis Onel, Dr. Baris Burnak, and Dr. Burcu Beykal were greatly appreciated.

The kind support of members of the Parametric Optimization and Control research group, members of the Mary Kay O'Connor Process Safety Center, and numerous others encountered along the journey is gratefully acknowledged.

CONTRIBUTORS AND FUNDING SOURCES

Contributors

This work was supported by a thesis committee consisting of Professors Efstratios N. Pistikopoulos, Mahmoud El-Halwagi, Joseph Sang-Il Kwon of the Artie McFerrin Department of Chemical Engineering and Professor Sergiy Butenko of the Department of Industrial and Systems Engineering.

All other work conducted for the dissertation was completed by the student independently.

Funding

This research was funded by the Mary Kay O'Connor Process Safety Center, the Texas A&M Energy Institute, and made possible in part by the National Institutes of Health (NIH) under award number P42-ES027704. The content of this work is solely the responsibility of the author and does not necessarily represent the official views of the NIH. Further, NIH does not endorse the purchase of any mentioned commercial products or services.

TABLE OF CONTENTS

LIST OF TABLES

Page

LIST OF FIGURES

Page

1. INTRODUCTION

1.1. Overview and Motivation

Maintenance refers to proximate acts undertaken to improve the availability of productive systems. These activities may include monitoring, inspection, cleaning, lubrication, testing, repair, or replacement depending on requirements. In a more general sense, maintenance is at the nexus of the broader concepts of system effectiveness and system resilience.

Maintenance can improve both system effectiveness and system resilience however system disruptions and a number of other challenges can lead to catastrophic over-maintenance or under-maintenance. Maintenance was seen to be a significant factor in 44% of process safety incidents examined out of which 69% were related to deficient planning, scheduling, and failure diagnosis [1]. Process safety incidents can lead to highly undesirable lost production as well as loss of containment of process fluids and a number of consequences that include: immense cost to human life, destruction of physical company assets, damage to intangible assets such as reputation, as well as negative impacts on the environment.

Research aimed at significantly reducing the likelihood of process safety incidents and system disruptions is thus of opportune interest. This research focuses on developing holistic approaches to inform decision-making. It leverages machine learning and mathematical optimization for data-driven maintenance planning, scheduling, and control toward improving the effectiveness and resilience of productive systems.

1.2. Challenges

Maintenance has a number of associated challenges which are presently outlined.

Challenge I: production systems are often dynamic, uncertain, complicated, and large. This is worsened by the complexities in failure mode behavior and by how safety is an emergent property of systems. Furthermore, decision multiplicity is prevalent given that systems can involve a large number of activities and resources. As such component criticality and resource prioritization is rendered non-trivial.

Challenge II: interactions between process conditions and maintenance of system components exist, are numerous, and can be nonlinear. This results in systems being challenging to model and control and high-fidelity first-principles models are intractable for many applications. Systems can also have rapid dynamics, require rapid automation for operability, and require non-overly-aggressive control actions.

Challenge III: maintenance windows and are becoming increasingly shorter and less frequent with activities that are increasingly more tightly coupled. This exacerbates the challenge of accounting for uncertainty in equipment condition that can result in increases in the mean time to repair. Furthermore, there are constraints on the amount, availability, and speed at which skilled workers can be attained.

Challenge IV: maintenance intrinsically results in competing objectives, and models traditionally used to plan maintenance have assumptions and employ uncertain parameters. This can lead to maintenance plans that are inaccurate and under-maintenance or over-maintenance. Furthermore, planning resource allocation is constrained and often exhibits diminishing marginal returns.

1.3. Research Opportunities

A number of research opportunities were identified after surveying the literature. The selected focus areas are summarized below.

Opportunity I: optimal prescriptive maintenance involving optimal future failure prediction and maintenance scheduling remains underexplored. Furthermore, consideration of the added dimension of process safety in prescriptive maintenance represents a significant research gap.

Opportunity II: active optimal control incorporating process and maintenance real-time optimization trajectories and schedules is an open question in the literature.

Opportunity III: large-scale optimal turnaround scheduling under resource constraints and uncertainty model parameters has witnessed limited exploration.

Opportunity IV: optimal resource-constrained maintenance planning considering uncertainties in reliability models and the effect of imperfect maintenance actions represents an area to make contributions.

Related research opportunities in chemical engineering not selected here include the following: failure prediction with reinforcement learning, grey-box maintenance scheduling, predictive plant-wide interdependent future failure propagation. Research opportunities identified in the surrounding related research fields of computer science, statistics, and industrial systems engineering not selected here include: uncertainty analysis of predictive algorithms outputs, and hierarchical classification using ensemble models.

1.4. Research Objectives

In light of the need for effective maintenance and process decision-making at multiple timescales, and recognizing the existence of multiple research opportunities, the present research proposes the following research objectives.

Objective I: Develop a future-fault-aware maintenance scheduling model to maximize system effectiveness and system resilience. This objective involves the development of ensemble support vector machine classification models for future failure prediction, and multi-objective scheduling of maintenance and process operations.

Objective II: Develop and implement an approach to explicit maintenance-aware failure-aware predictive control. This objective involves the integration of real-time optimization, dynamic simulation, machine learning, and multi-parametric model predictive control.

Objective III: Develop a scheduling model to optimize turnarounds subject to workforce constraints and repair time uncertainty. This objective involves the use of mixed-integer stochastic programming and reinforcement learning.

Objective IV: Develop a multi-objective stochastic maintenance planning model. This objective involves the consideration of an effective equipment age model and uncertainty in reliability model parameters for maintenance capacity planning.

1.5. Paradigm

Maintenance and production are interrelated and exhibit dynamic interactive complexity which leads to a number of identified research challenges, opportunities, and objectives.

This dissertation operates within a holistic paradigm that seeks to optimally improve the system effectiveness, system resilience, and sustainability of integrated operations. This is termed the Safety-Aware SUstainable MAintenance and Process optimization (SASUMAPRO) paradigm and is shown in Figure 1. Elements of this paradigm are subsequently demonstrated in turn throughout the rest of this dissertation.

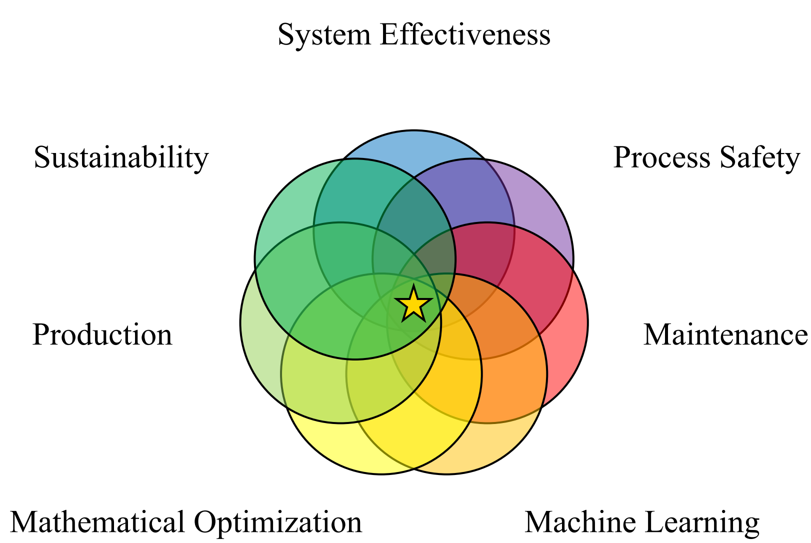


Figure 1: SASUMAPRO paradigm

2. BACKGROUND

This research involves several different concepts and an attempt has been made to provide background information to help readers contextualize and fully appreciate the present research. This section discusses a subset of essential related concepts in: (1) system effectiveness, (2) process safety, (3) maintenance, (4) machine learning, and (5) mathematical optimization. The chapter then concludes with a generalized and holistic safety-aware sustainable maintenance and production model that links these concepts together.

2.1. Systems Effectiveness

System effectiveness is the holistic performance of a system as a function of its availability, reliability, and quality characteristics [2]. System effectiveness can be applied to individual equipment or extended to a multi-component process system. It is noted that system effectiveness is function of equipment effectiveness. System effectiveness considers various performance characteristics: availability, which characterizes the probability that a piece of equipment will be available at a given time; productivity, which relates to the profitability of the process as a function of its production rates; and quality, which serves as a lagging indicator by characterizing whether products meet standards. It is noted that the cost of low availability, low productivity, and poor quality can all be quantified in monetary terms.

The factors influencing performance characteristics are interdependent, which leads the performance characteristics to be interdependent. For example, an effective predictive maintenance program resulting in fewer equipment breakdowns concomitantly would result in higher production rates and better product quality. This example illustrates process-maintenance interactions, as well as how the presence of high availability can help enable high productivity. This then motivates and shows the value of a systematic approach that considers the various interdependent factors in a systematic and holistic fashion.

System effectiveness quantification is key as it enables a number of different technical and organizational aspects: (1) real-time assessment of performance, which involves tracking and online performance benchmarking against set standards; (2) incorporation of and augmentation of multiple interdependent considerations within a single metric; (3) consideration of the expected system performance in a probabilistic aspect to avoid making conclusions that are based on deterministic single point values; (4) priority management and guided resource allocation for continuous improvement through equipment criticality assessment; as well as (5) ready communication of performance to multiple stakeholders.

The utility of system effectiveness as well as system effectiveness quantification is well-established and one of its earliest specific formalizations comes from total productive maintenance [3]. Total productive maintenance defines overall equipment effectiveness as a function of availability, productivity and quality. System effectiveness is often formalized as a product or unweighted geometric mean of availability, productivity, and quality [4]. However it can also be considered as a weighted arithmetic mean using summations. It is noted that system effectiveness can alternatively be considered as a multi-objective problem and formalized using methods such as: epsilon-constrained method, analytic hierarchical process, multi-attribute utility theory, Bayesian networks. While many objective functions can be cast as partial system effectiveness metrics, a select few of them relate to maintenance and production optimization at different time scales. These objective functions are summarized in Table 1.

Table 1: Partial overview of system effectiveness objective functions

Reference	Objective Function
[2] [5] [6]	**Profit**
[7]	**Cost**
[8]	**Production Equipment Effectiveness (PEE)** $\text{PEE} = \text{Availability}^{k_1} \times \text{Efficiency}^{k_2} \times \text{Quality}^{k_3}$
[9]	**System Survivability Index (SSI)** $\text{SSI} = \left(\frac{\text{Actual System Effectiveness}}{\text{Required System Effectiveness}}\right)$

2.2. Process Safety

Process safety is a field of research that involves prevention, mitigation, and response to dangers associated with industrial processes. The dangers of industrial processes are termed hazards. A hazard is defined as a chemical or physical condition that can potentially cause damage to people, property, or the environment [10]. The level of safety of a process containing hazards is known as risk. Risk is defined as a measure of both the probability and severity of human injury, economic loss, or unsustainable environmental damage due to process safety incidents that include fire, explosion, or toxic release. Process operators collect various types of data to help understand process risk. These can be summarized in a safety data pyramid [11] as shown in Figure 2.

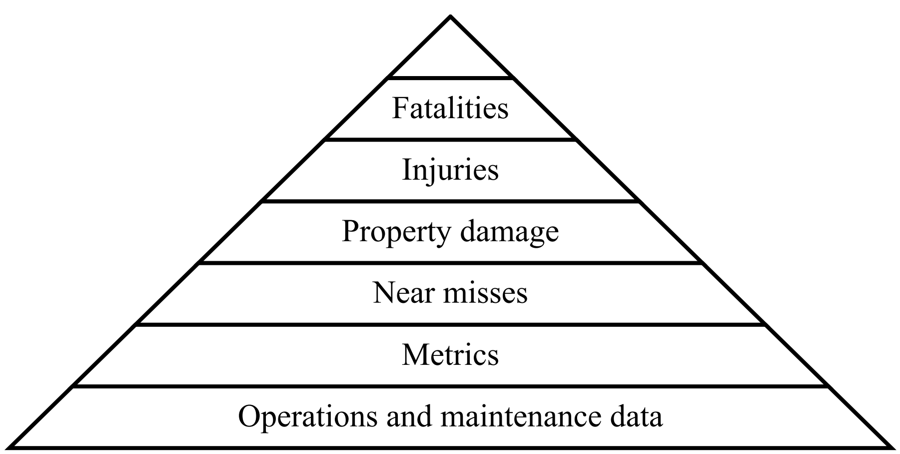


Figure 2: Safety data pyramid

It is noted that each level of the safety data pyramid can be leveraged help improve process safety. Operations and maintenance data can be analyzed to improve system effectiveness, however it suffers from high variety, high velocity, high volume, and low veracity which motivates the use of big data and machine learning techniques. Metrics can be constructed from operations and maintenance for performance benchmarking. Near misses are defined hear as an opportunity to learn from a near hit or potential catastrophic incident. Loss of containment of process fluid and asset damage are defined here as property damage and not near misses. The pyramid is capped by data on injuries and fatalities.

It can be observed that the lower levels of the safety pyramid is are characterized by significantly more abundant data than the higher levels of the safety pyramid. Data from the lower levels can serve as leading indicators [12] for compromised process safety, however these warning signs may be weak signals and are not always comprehensible [13]. Research that deciphers safety data effectively to anticipate and avoid incidents is thus of value.

Risk assessment methods aim to leverage this safety data to quantify and explain process safety performance using a variety of methods. These risk assessment methods can be categorized as: (1) qualitative, through the use of what-if analysis, checklist, failure modes and effects analysis, as well as hazard and operability studies; (2) semi-quantitative, with methods such as layer of protection analysis; or (3) quantitative, with methods that include fault trees and dynamic fault trees, event trees and dynamic event trees, bowtie analysis, Bayesian networks and Dynamic Bayesian networks, as well as safety metrics [10].

Traditional conducted risk assessment can experience a number of limitations. These include it being: complex, costly to calculate, time-consuming, often static, often purely qualitative, as well as often narrow in scope to not effectively account for interactions and socio-organizational factors. Effective use of safety data could help by improving both the consequence modeling and probability modeling aspects of risk quantification.

Consequence modeling involves the use of first-principles or data-driven models to simulate aspects of process safety incidents and calculate the magnitude and spread of their damage [14]. It is driven by safety data and examples of software to perform consequence modeling include: ALOHA, PHAST/CANARY, and FLACS. In performing consequence modeling key considerations include: location; the type of failure; the type of chemicals; and atmospheric conditions such as temperature, humidity, wind speed, wind direction, wind stability class [10, 14]. Consequence modeling can be computationally challenging and significantly affected by epistemic uncertainty however safety data can help improve model accuracy.

Probability modeling quantifies the likelihood of a process safety incident. However processes are highly complex and determining whether a piece of equipment will fail, and going beyond that to quantify the probability of occurrence is rendered non-trivial and highly challenging. This leads to a significant amount of uncertainty in the probability side of risk. Given that several aspects of operations and maintenance impinge upon process safety, approaches that can tackle the holism, complexity, and operability of process systems are key.

One such method is Bayesian networks. Bayesian networks are directed and acyclic graphs that can be used to represent the complex probabilistic relationships in systems with interdependent components [15]. Bayesian networks are composed of two structural components: nodes and edges. Nodes represent the random variables corresponding to system components whereas edges represent the relationships between the system components. Commonly used terminology to describe Bayesian networks include: parent nodes, the nodes from which the directed edges emanate; child nodes, the nodes to which edges are directed; static, non-time-varying Bayesian networks; and dynamic, Bayesian networks in which the influence of past nodes is propagated through the network over time.

It is noted that Bayesian networks assume that child nodes are assumed to only depend on their most proximate parent nodes [15]. It is further noted that as opposed to fault trees which primarily use combinations of AND gates and OR gates, Bayesian networks use Bayesian inference to determine the probability distribution of each child node given the probability distributions of their parent nodes [15]

An example of a Bayesian network is presented in Figure 3. It depicts child nodes (I, J) that characterize the safety of a system that is influenced by parent nodes (X, Y, Z), over two discretized time intervals (T1, T2). The Bayesian network depicted in the example is relatively simple, however for complex systems the mathematics of Bayesian networks becomes highly challenging.

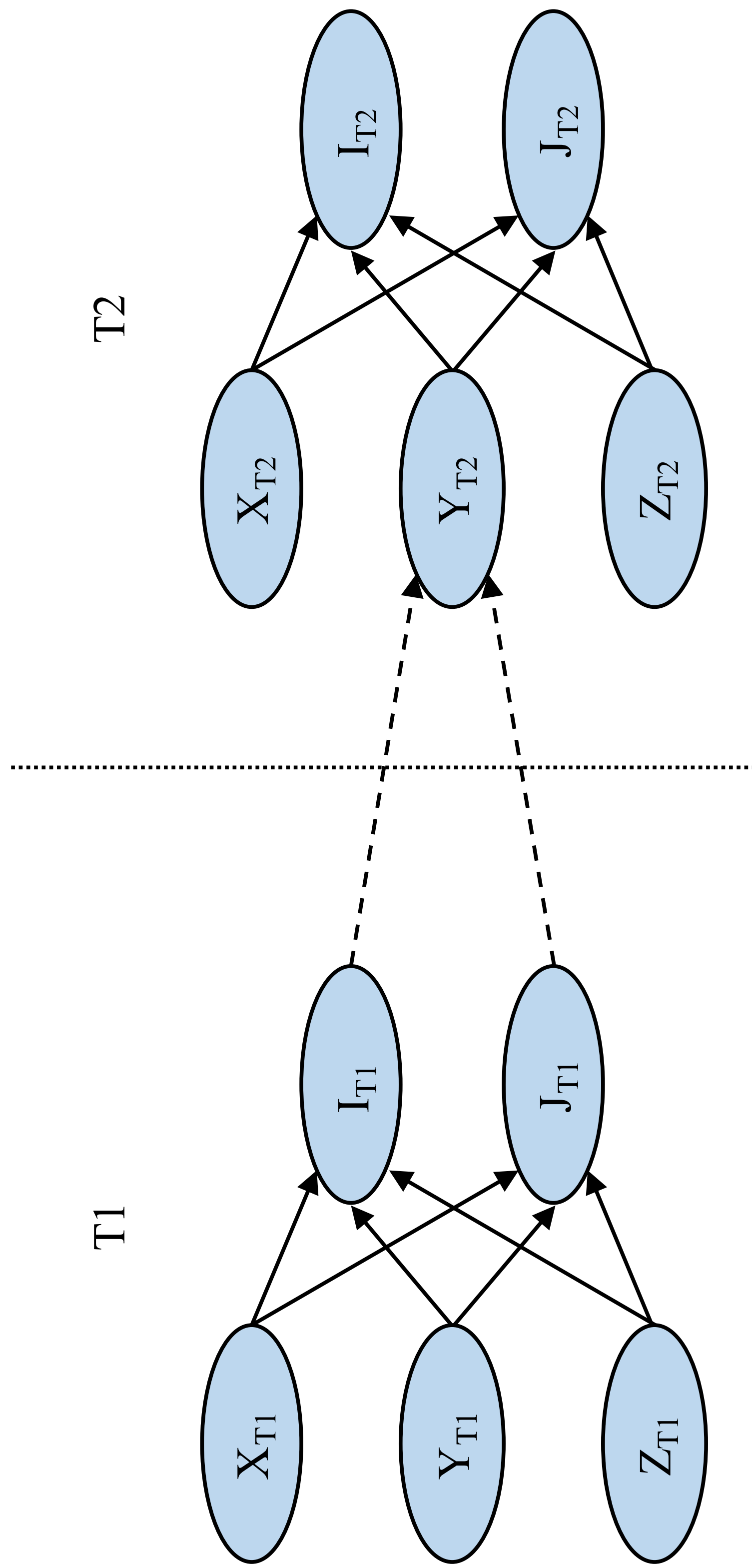


Figure 3: Dynamic Bayesian network

One alternative approach that is commonly thus used is safety metrics due to their lower computational requirements relative to other quantitative risk assessment models. The safety metrics are key performance indicators (KPIs) that aggregate individual measured indicators to quantify the state of systems that [12]. Safety metrics are of interest because they enable one to: (1) track, analyze, and assess the health of barriers in the system as well as to monitor asset productivity; (2) anticipate and avoid process safety incidents and their consequences; (3) make system states observable so as to take decisions and assist with communication to all stakeholders.

Safety metrics employed should incorporate some knowledge of failure modes [16]. As such systematic approaches need to be taken to develop representative safety metrics. These approach should consider various aspects provided in Table 2. Safety metrics also enable benchmarking so as to improve future performance against internal targets, and competitors. Safety metrics also help ensure compliance with regulatory standards which in effect represent mandatory mathematical constraints on operations and maintenance.

One such standard that in effect summarizes process safety is known as the Occupational Safety and Health Administration (OSHA) Process Safety Management (PSM) standard [10]. This standard contains information related to the 14 process safety elements shown in Table 3 [10]. Maintenance falls under the element of mechanical integrity and requires understanding of the other elements to be done effectively.

Table 2: Categorization of aspects of safety metrics and indicators

Category	Aspects
time	static dynamic
horizon	lagging leading
scale	equipment unit facility company industry
quality	quantitative semi-quantitative qualitative
type	technical non-technical
life-cycle segment	design operations

Table 3: PSM elements

#	**Element**
1	Process safety information
2	Process hazard analysis
3	Operating procedures
4	Employee participation
5	Training
6	Contractors
7	Pre-startup safety review
8	Mechanical integrity
9	Hot work permit
10	Management of change
11	Incident investigation
12	Emergency planning and response
13	Compliance audits
14	Trade secrets

2.3. Maintenance

Maintenance in an abstract sense refers to sustaining the availability of equipment by improving their ability to resist destructive stresses within their material continua. More concretely maintenance takes the form various actions which include: cleaning; inspection through online, or offline assessment of equipment; testing, to physically stimulate equipment to assess performance and integrity; repair; as well as replacement. Here maintenance and mechanical integrity are used synonymously due to their large degree of overlap. With process-maintenance interactions, increases in the resilience of individual equipment can simultaneously improve system resilience and can also improve system effectiveness.

The objective of maintenance departments has traditionally been equipment mechanical integrity. Over time, a number of maintenance programs have emerged. These are also termed maintenance policies or maintenance philosophies and include: risk-based inspection, in which risk-based criticality analysis is performed to prioritize which equipment to maintain; total productive maintenance, which places a greater focus on the socio-organizational interactions between production and maintenance; as well as reliability-centered maintenance, which explicitly places reliability at the core of maintenance decision making.

One of the primary ways that maintenance departments obtain information is through inspections. Inspections of equipment are done to: assess current state of equipment, by checking factors such as damage and alignment; assess performance of equipment; assess rate of degradation; as well as to perform root cause analysis of condition degradation or performance degradation. Inspections generally involve taking the equipment offline, however techniques such as visual inspections, unusual odor detection, and vibration analysis can be used to perform online inspections [13]. Inspections are carried out on a periodic basis at intervals that depend on type of equipment, their criticality, standards, and recognized and generally accepted best engineering practices. One challenge however is that inspections are often done on an arbitrary time basis such as the following: every three months for pumps, every six months for process valves, yearly for piping, and yearly for relief valves. It is emphasized that the specific intervals provided here are arbitrary.

Mechanical integrity programs can suffer from a number of other known challenges which include: difficulties in tailoring the specific practices and procedures at individual sites to general standards, siloing of mechanical integrity responsibilities to only the maintenance department of companies, improper documentation and management of maintenance procedures, as well as expired or undocumented qualifications for maintenance technicians [17].

These challenges often result in reduced effectiveness of maintenance activities and poorly performing maintenance. Key maintenance performance metrics [13] include: work orders completed as a percentage of scheduled work orders; overall equipment effectiveness; availability; downtime vs uptime; total maintenance cost relative to budget; planned maintenance percentage vs total maintenance; ratio of planned to unplanned maintenance; maintenance cost per unit; extent of technician training; as well as personal safety metrics such as total recordable incident rate and lost workday rate. Maintenance programs also track a set of lagging indicators [12] which include: mean time to repair; mean time between failures; maintenance response time; personnel utilization; percentage of rework work orders [13].

As a result of the challenges of mechanical integrity programs, the current philosophy that is beginning to come become predominant and wide-spread is condition-based monitoring, in which maintenance is centered around measurements of the condition of equipment over time. Condition-based monitoring typically refers to measurements directly related to equipment health. A partial overview of typical measurements present in condition-based monitoring is provided in Table 4.

Regardless of the underlying maintenance philosophy and mechanical integrity program, one central element is maintenance decision-making. This refers to the specific basis and techniques used to decide whether or not to take a piece of equipment offline for maintenance. Traditionally three archetypes have been used to categorize maintenance decision-making namely: (1) corrective, (2) preventive, and (3) predictive. Here the following six archetypes are proposed to nuance and categorize maintenance decision-making approaches: (1) corrective, (2) fixed interval-based, (3) preventive, (4) condition-based, (5) predictive, and (6) prescriptive. The decision tree categorizing these archetypes is displayed in Figure 4 and the archetypes are presented in Figure 5.

Table 4: Partial summary of condition measurements for different equipment

Equipment	**Measurements**
Pumps	visual check of seals performance (ex. pressure) abnormal vibration bearing oil temperature bearing oil composition abnormal noise
Heat exchangers	visible fouling temperature difference pressure drop product composition ultrasonic
Towers	visible damage to internals electrochemical thickness external infrared thermography internal temperature profile level pressure profile
Vessels	visible cracks ultrasonic electrochemical thickness painting
Valves	acoustics actuation time seal temperature
Piping	electrochemical thickness external infrared thermography pressure profile
Instrumentation	latency power

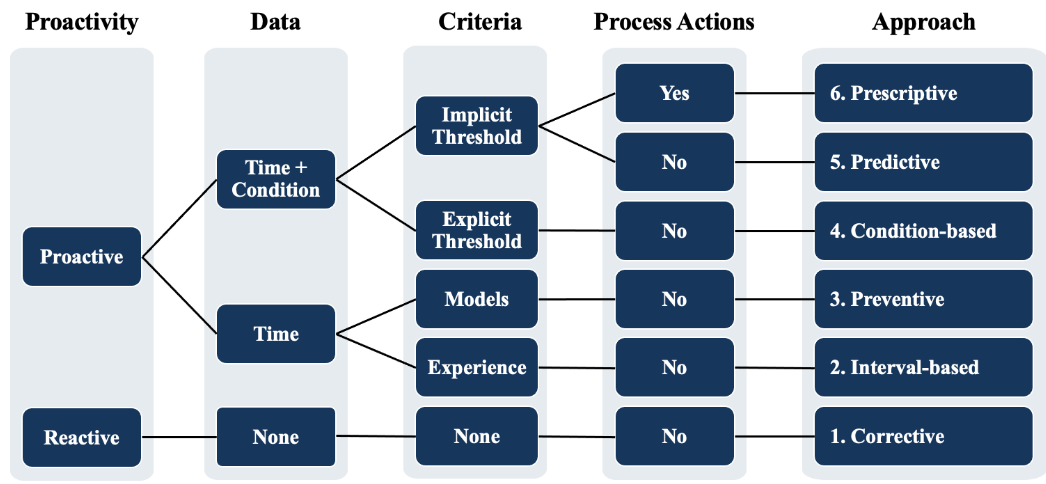


Figure 4: Maintenance decision making approach classification

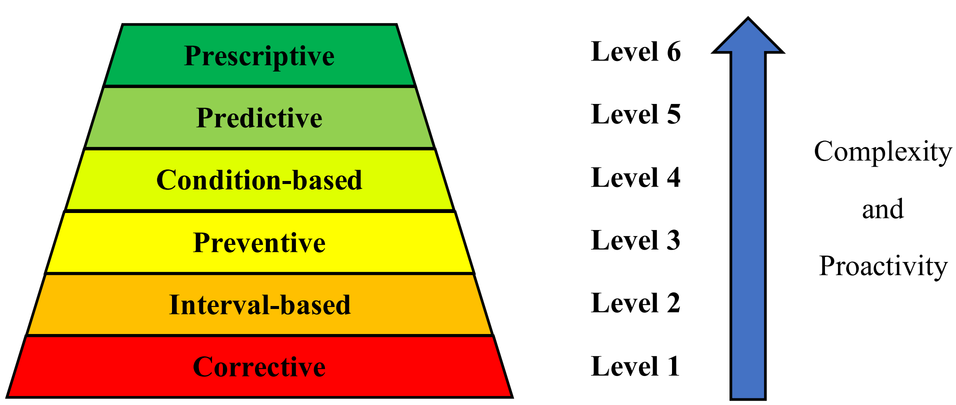


Figure 5: Maintenance decision making approaches

These maintenance decision-making approaches are organized into six corresponding levels based on the degree of complexity and proactivity that they contain. It is noted that different levels have fuzzy interfaces with some specific techniques falling into two contiguous approaches. Different approaches may be more or less suitable for different pieces of equipment according to their criticality, and service. It is further noted that risk analysis and cost-benefit analysis can be employed in selecting a maintenance decision-making approach.

The maintenance decision-making approaches are presently described. In corrective maintenance, the decision-making is relatively absent and maintenance actions are based on allowing equipment to fail before fixing them. In fixed interval-based maintenance, fixed time intervals are used to determine when to perform maintenance actions. Traditionally used inspection intervals are an example of interval-based maintenance. Preventive maintenance decision-making approaches represent a marginal step up in complexity and involve the use of mean time between failure data to derive two or three parameter reliability models. An example of a preventive maintenance decision-making approach is the use of Weibull-type analysis [18].

Condition-based maintenance leverages measurement of equipment condition obtained from condition-based monitoring programs to decide when to do maintenance. This decision is typically based on explicit univariate thresholds that are either set based on best judgement, or calculated according to physics-based equations. An example of condition-based maintenance is tracking the thickness of a pipe wall over time and then replacing the pipe once the pipe thickness falls below say 75 % of the original thickness so as to avoid loss of pressure resistance imparted by material strength leading to a rupture and loss of containment.

It is noted that the service, operating conditions, and chemical composition of fluids in process equipment could change significantly over long periods of time leading to inaccuracies in applying previously determined original equipment manufacturer maintenance recommendations or historical condition-based thresholds.

Predictive maintenance leverages machine learning algorithms to decide when to do maintenance based on condition data, time data and other types of data. It is noted that in effect predictive maintenance decision-making approaches typically tend to extract an implicit condition threshold, and that this threshold is based on measured data.

Predictive maintenance has a number of advantages. The underlying advantage is that it avoids arbitrariness by offering *data-driven* decision-making capability that is *customized* to equipment based on their specific health, service, and environmental condition. From a business perspective, the advantages of effectively implemented predictive maintenance are summarized in Table 5. It is noted that predictive maintenance is highly reliant on data availability and data veracity, however well digitalized operations and maintenance supports the key advantage of predictive maintenance to be able to dynamically estimate explicit as well as implicit future degradation profiles.

Table 5: Advantages of predictive maintenance

Category	**Advantage**
Time	reduced equipment downtime increased availability
Cost	decreased number of process safety incidents and emergency situations decreased labor cost
Quality	reduced risk to customers of compromised service quality improved product quality
Human factors	increased personnel satisfaction better utilization of personnel.
Socio-organizational factors	improved spare part inventory management data-driven decision-making

Table 6: Partial summary of process measurements

Approximate Type	**Measurements**
Mass	metal debris mass average catalyst mass
Amount	gas content chemically-attacking species concentration
Temperature	process fluid temperature ambient temperature cooling water temperature heating oil temperature steam temperature
Length	average machine arm displacement machine odometer readings semiconductor feature size variability pipeline position
Current	current Fourier spectra root-mean-squared voltage
Time	start-up sequence load spikes times time since last maintenance absolute operational time relative operational time
Luminosity	solar irradiance filament brightness
Force	pressure friction viscosity material stress
Nondimensional	efficiency inlet-to-outlet flow ratio stress-strain ratio speed ratio

Prescriptive maintenance builds upon the advantages of predictive maintenance by additional consideration of process decisions and their effect on equipment and system failure. Prescriptive maintenance is prediction *plus* action and it leverages process measurements to a significantly greater extent. A partial list of relevant process measurements can be found in Table 6.

Optimal prescriptive maintenance goes a step further to take a holistic approach that leverages state-of-the-art machine learning and rigorous mathematical optimization techniques to simultaneously maximize system effectiveness and the level of system resilience. As such, optimal prescriptive maintenance has the capability to account for the nonlinear interactions of process, maintenance, and the environment while simultaneously recommending the optimal process actions to achieve a precise balance between risky under-maintenance, costly over-maintenance, and production.

Optimal prescriptive maintenance thus enables decision makers to determine the best maintenance *and* operational decisions to take for their systems. These decisions include: the maintenance schedule; the process operating schedule; turnaround duration; turnaround frequency; personnel-equipment task assignment; maintenance action type task execution; process operating conditions; capacity allocation for maintenance planning; as well as spare-part management. Optimal prescriptive maintenance also offers the ability to rigorously consider constraints whether they be: constraints on resources required such as utilities, cranes, fork-lifts, and labor; constraints on safety; constraints from regulations; or process inequality and equality constraints.

2.4. Machine Learning

Machine learning is a field within artificial intelligence research that focuses on developing data-driven models and algorithms. As opposed to first-principles methods, in machine learning the models do not necessarily have a structure that is known *a priori* but rather have the flexibility to learn model structures from data to be able to capture complex physical phenomena such as those that can lead to process safety incidents. As a result there has been growing excitement and interest in machine learning within the chemical engineering community due to its promise in tackling long-standing and highly challenging problems [19]. This dissertation focuses on two such challenging problems in the context of data-driven maintenance optimization: failure prediction, and fault detection.

There are three main paradigms in machine learning: (1) supervised learning, (2) unsupervised learning, and (3) reinforcement learning [20]. Supervised learning deals with columns of data known as features that are each labeled and uses them to predict binary outcome vectors through classification methods as well as to predict continuously-valued outcome vectors through regression methods. Unsupervised learning in contrast deals with data that may not be labelled and has primarily focused on identifying underlying clusters of data with models such as include k-means, k-nearest neighbors, and hierarchical clustering. Reinforcement learning can be conceptualized as data-driven optimization and involves the use of algorithms as agents that learn which optimal actions to implement within an environment to maximize a mathematical reward with algorithms such as Q-learning, and generative adversarial networks.

Machine learning is leveraged by the present research for disruption prediction and this is done through a systematic workflow that consists of a number of steps.

1. Feature measurement: involves leveraging an established digital data collection infrastructure to sample operations and maintenance processes. This data include: time measurements such as age, days elapsed since last maintenance, and days elapsed since last failure; condition measurements such as vibration, temperature, and composition; as well as process measurements such as rate, voltage, and power.

2. Feature generation: then involves transforming features to engineer new features using physics-based engineering judgement or statistical techniques. Generated features can include calculated physical quantities, characteristic dimensionless numbers, features that capture absolute deviations from baselines, and lag features that are measurements from previous time steps. Feature generation techniques [20] include: normalization, via taking ratios of features, min-max scaling, and *Z*-transformation; aggregation to combine multiple data points via calculating quantities such as the rolling mean, median, min, max, and standard deviation; signal processing which involves determination of wavelets, root mean square, frequency domain transformations, and skew [21]; features from dimensionality reduction through principal components analysis; as well as discretization to replace continuous-valued data with class labels corresponding to different bins.

3. Feature selection: involves the use of heuristics, algorithms, and techniques to reduce the number of features to the most useful subset for developing models. There are two primary categories of feature selection methods: (1) filter-based methods which select features independently of models, and (2) wrapper methods which select features using algorithms embedded within model creation algorithms. Filter-based methods include: correlation analysis, and mutual information computation [22]. Wrapper methods include genetic-based algorithms, exhaustive feature selection; and sequential search over subsets of features [22].

4. Model creation: involves the use of algorithms to learn the structure of models from data and determine values of the model hyperparameters. Model creation intrinsically involves parsing the hyperspace of parameter values to optimize objectives such as prediction error. It is noted that various models can be adapted for use for either classification or regression. Classification models include support vector machines, decision trees, naïve bayes classifiers. Regression models include random forest, neural networks, and lasso regression. In the context of failure prediction and fault detection, the created models learn the ways that faults and failures affect the feature values. In a sense the created models can thus learn the dynamics of the system and the difference between normal operating conditions and many abnormal operating conditions.

5. Model tuning: then involves refining the optimized hyperparameters to improve the performance of the model. This is typically done via two ways: (1) grid search, in which a model is created for each combination present in the superset of discretized hyperparameter values; and (2) optimization, in which typically metaheuristic algorithms are used to iteratively obtain hyperparameter values that improve model performance.

6. Model evaluation: involves assessing the performance of the model. It is noted that the model training and model tuning steps involve some intrinsic assessment of performance, however this is done on the data used to build the model. Model evaluation on the other hand is used here to refer to testing the model on data that was not used to create it so as to obtain a better sense of its generalizability and likely performance.

7. Model deployment: represents the last step of the workflow and involves implementing the model for decision support. Model deployment typically involves feeding real-time data into the model to obtain insights. It is noted that stakeholders should be consulted at all stages of the workflow prior to deployment to help ensure buy-in and successful value creating deployment.

Support vector machines represent one type of model used extensively in this dissertation and is thus explained in slightly more detail for the reader's convenience. Support vector machines, in the context of classification, are models constructed from historical data that assign class labels to new input data.

The underlying principle of support vector machines for classification is that data can effectively be transformed into a hyper-dimensional feature space to better discern class membership [23]. For binary classification, historical data is first labelled with +1 or -1 to describe sample class membership. The labelled historical data is then effectively transformed into a hyper-dimensional feature space using a selected kernel function, and then used to obtain the optimal hyperplane that separates the data such that the majority of samples belonging to different classes are on opposite sides of the separating hyperplane. The process of obtaining the optimal hyperplane involves formulation of the machine learning problem as a mathematical optimization problem, deriving the corresponding dual formulation, and then solving the resulting convex optimization problem to global optimality. In the model deployment step, class membership of a new input data point is assigned by determining which side of the hyperplane the data point falls.

2.5. Mathematical Optimization

It is of great interest to optimize maintenance decision-making so as to minimize cost and maximize system effectiveness to help improve overall system resilience. Mathematical optimization is a field of research that employs mathematical models of systems, and algorithms, to obtain optimal solutions to problems to assist with decision-making. Specifically, mathematical optimization refers to modeling using equations, inequalities, and algorithms to take the binary, integer and/or continuous decisions that cause objective(s) to take on their optimal value. This research leverages a number of different types of optimization including: (1) stochastic optimization, (2) integer programming, (3) nonlinear programming, and (4) multi-objective optimization. Each of these is summarily described.

Stochastic optimization involves consideration of uncertainty in the parameters used in optimization models. This is in contrast with deterministic optimization in which the parameters are treated as being known with certainty. One type of stochastic optimization used here is known as scenario-based stochastic programming in which the probability distributions of the random variables are approximated using discrete distributions [24]. Consider the average price of electricity as an optimization model parameter for example: deterministic optimization would treat it as being a known fixed value of say $0.12/ Kwh, whereas scenario-based stochastic programming would treat it as being an uncertain distributed value by introducing different scenarios characterized by a value vector of say [$0.10, $0.12, $0.15] with concomitant realization probabilities of [30%, 40%, 30%]. It is noted that there are other stochastic programming methods that involve the use of chance constraints, and fuzzy logic [24]. It is further noted that scenario-based stochastic programming typically leads to larger and more challenging optimization problems. In the context of multi-period problems especially, this imparts a significant degree of additional solution complexity leading to the necessity of leveraging extensive computational resources, scenario reduction algorithms, or iterative bilevel algorithms.

Integer programming involves the use of binary variables and algorithms to more readily formulate and solve optimization problems that exhibit discrete decisions. An example of a discrete decision is whether or not to perform maintenance on a centrifugal pump within a given time interval. Integer programming is facilitated with the use of propositional logic which systematically encode the different logical relations between different propositions corresponding to binary variables into inequalities. It is noted that the space of different discrete decision combinations can be exponentially large and that inequalities such as integer cuts, and algorithms such as branch and bound [25] enable intelligent parsing of the discrete decisions spaces so as to avoid the computational intractability associated with exhaustive enumeration.

Nonlinear programming involves the reformulations and algorithms to seek global optima. Nonlinear functions can exhibit optima multiplicity and nonlinear programming specifically seeks rigorous ways to help optimization algorithms escape local optimal to find the best overall solution in the decision space. This is traditionally done by creating surrogate functions known as convex envelopes to approximate the nonlinear functions. One such convex envelope is known as the

McCormick relaxation [25]. It is noted that an awareness is needed of the domain of the functions in relation to the maximum separation distance between the convex envelopes and the original nonlinear functions. It is further noted that methods such as stochastic gradient descent can be used for nonlinear programming problems to obtain good feasible solutions.

Multi-objective optimization involves the systematic solution of problems that simultaneously involve multiple and possibly competing objective functions. This is formalized through the field of multi-objective optimization with a general form shown in (1).

$$\begin{aligned} \min_{\mathbf{x},\ \mathbf{y}} \quad & \mathbf{f}(\mathbf{x},\mathbf{y}) = [\mathrm{f}_1(\mathbf{x},\mathbf{y}), \mathrm{f}_2(\mathbf{x},\mathbf{y}), \dots, \mathrm{f}_\mathrm{N}(\mathbf{x},\mathbf{y})] \\ \text{s.t.} \quad & \mathbf{g}(\mathbf{x},\mathbf{y}) = 0 \\ & \mathbf{h}(\mathbf{x},\mathbf{y}) \leq 0 \\ & \mathbf{x} \in \mathbf{X} \subseteq \Re^{\mathrm{n}} \\ & \mathbf{y} \in \mathbf{Y} \{0,1\}^{\mathrm{m}} \end{aligned} \tag{1}$$

Multi-objective problems can be solved using a variety of methods. These include lexicographic goal programming, and the use of weighted-averaging. Weighted-averaging scales each objective function and then combines them via an arithmetic or geometric average into a single objective function that can be solved with standard methods. Weighted-averaging however suffers from uncertainty in selecting which weight factors to use and difficulty in interpreting different weight factor combinations. The epsilon-constrained method has consequently emerged as a way of tackling multi-objective problems [26]. This method is done by first solving the multi-objective problem using each objective function at a time without the other objective functions to help define narrow ranges for the objective functions. Each of the objective function ranges is then discretized to obtain all combinations of objective function values (E). A single objective function is then selected to be optimized for each combination subject to the other objective functions constrained by the obtained objective function values. The additional constraints that result from this method are known as ε-constraints ($\varepsilon \in E$). This is shown for a generic bi-objective optimization problem in (2).

$$
\begin{aligned}
\min_{\mathbf{x},\ \mathbf{y}} \quad & \mathrm{f}_1(\mathbf{x}, \mathbf{y}) \\
\mathrm{s.t.} \quad & \mathrm{f}_2(\mathbf{x}, \mathbf{y}) \leq \varepsilon \\
& \mathbf{g}(\mathbf{x}, \mathbf{y}) = 0 \\
& \mathbf{h}(\mathbf{x}, \mathbf{y}) \leq 0 \\
& \mathbf{x} \in \mathbf{X} \subseteq \Re^{\mathrm{n}} \\
& \mathbf{y} \in \mathbf{Y}\, \{0,1\}^{\mathrm{m}}
\end{aligned}
\tag{2}
$$

It is noted that correct application of the epsilon-constrained method results in a set of solutions called a Pareto front an example of which is shown in Figure 6. The solutions have the desirable characteristic of being nondominated, which means that selecting a different solution with a better value of one objective function results in a worse value of other objective function(s). In other words the solution to the transformed multi-objective problem is a set of optimal decision vectors that are true alternatives. The decision maker can then select from the solutions by trading off the alternatives qualitatively based on their desired criteria.

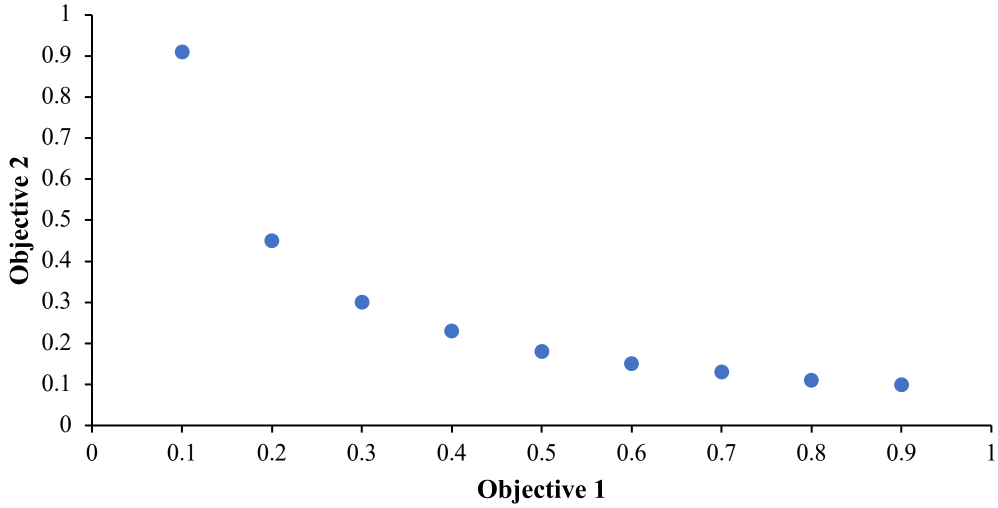


Figure 6: Pareto front of solutions to a multi-objective optimization problem

2.6. Generalized Model

Optimal prescriptive maintenance is consistent with the holistic paradigm and is at the nexus of system effectiveness, process safety, maintenance, machine learning, and mathematical optimization. These aspects can be combined into a generalized model with system effectiveness as an objective, process safety as an objective and constraints, as well as maintenance and production as constraints. Machine learning helps with quantifying fault and failure probability and mathematical optimization helps with obtaining decisions. This chapter concludes with the generalized model shown in Table 7.

Table 7: Safety-aware sustainable maintenance and production model elements

Facet	Elements
Objectives	system effectiveness system resilience sustainability
Process Model	mass balances heat balances reaction equilibrium relations utility balances process specifications product quality specifications demand constraints supply constraints storage and inventory constraints sequence constraints cycle time constraints logical constraints startup and shutdown constraints
Maintenance Model	concurrent maintenance constraints regulatory maintenance constraints inspection constraints cleaning time considerations repair time considerations equipment age constraints scheduled downtime constraints
Safety Model	probability quantification consequence quantification risk model structure
Sustainability Model	emissions model energy use products biodegradability considerations

3. LITERATURE REVIEW

3.1. Overview and Meta-Analysis

This section contains a summary of research related to data-driven maintenance planning, scheduling, and control. It begins with meta-analysis, and then continues with an indicative exposition of selected research efforts. These research efforts are categorized into the following research areas: (1) data-driven modeling, which focuses on the use of surrogate models for fault and failure prediction; (2) maintenance optimization, which spans optimal planning and scheduling; (3) process control, with emphasis on explicit model predictive control; and (4) process safety quantification, focusing on dynamic quantitative risk assessment.

Meta-analysis was performed using Web of Science on related topics in the literature. As reflected in Figure 7, publications related to optimization and involving the use of grey-box, surrogate, or data-driven models have seen a significant increase over time. This trend has been accompanied by an exponential explosion of interest in machine learning in recent years shown in Figure 8. Machine learning can be seen to span several research areas and has emerged to become a multinational phenomenon as evidenced in Figure 9 and Figure 10. Interestingly as seen in Figure 11 and Figure 12, predictive maintenance involving machine learning continues to grow exponentially and is poised to overtake the preceding saturating research area of preventive maintenance. The meta-analysis shows that research into maintenance involving data-driven models and machine learning is of worthwhile interest.

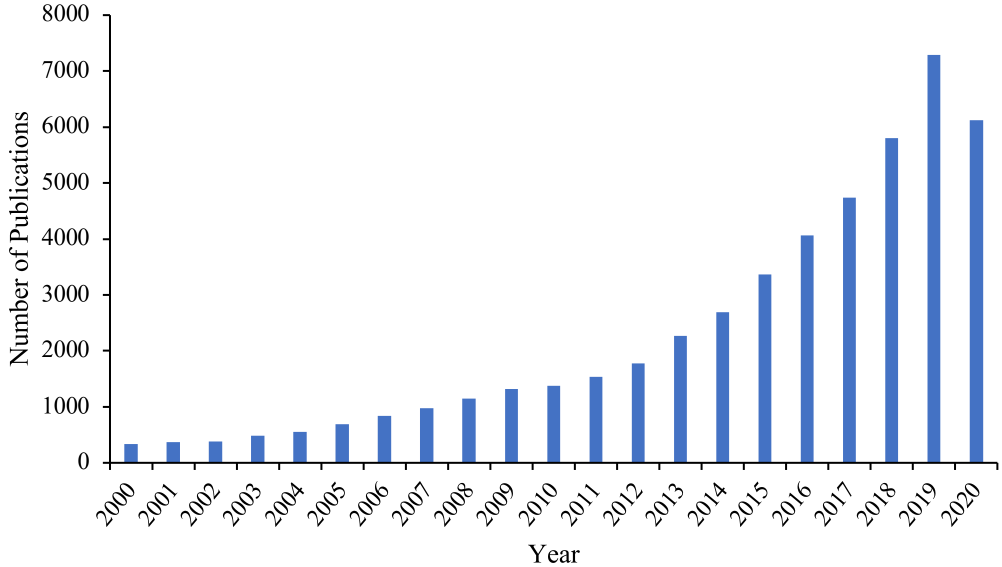


Figure 7: Data-driven modeling research publications over time

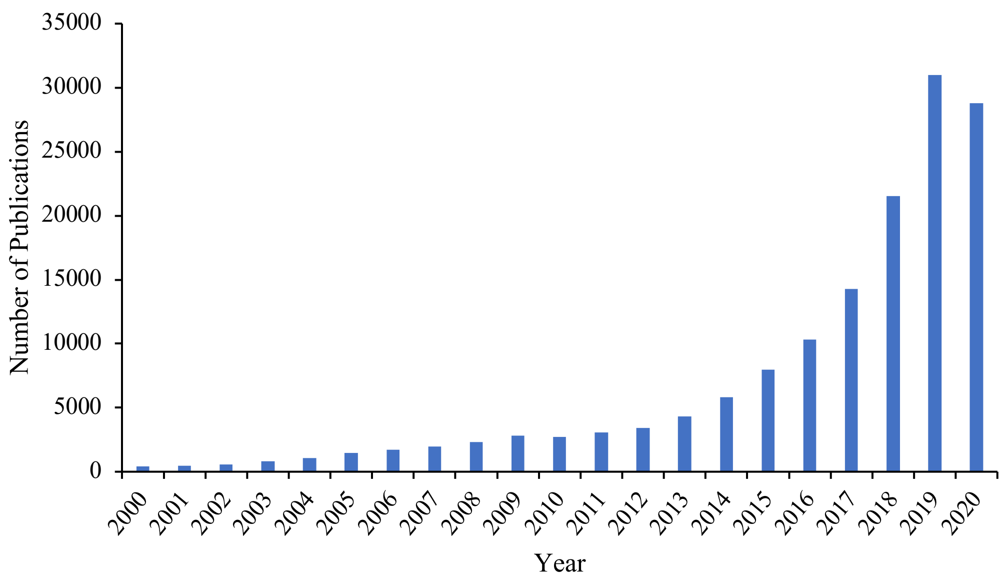


Figure 8: Machine learning research publications over time

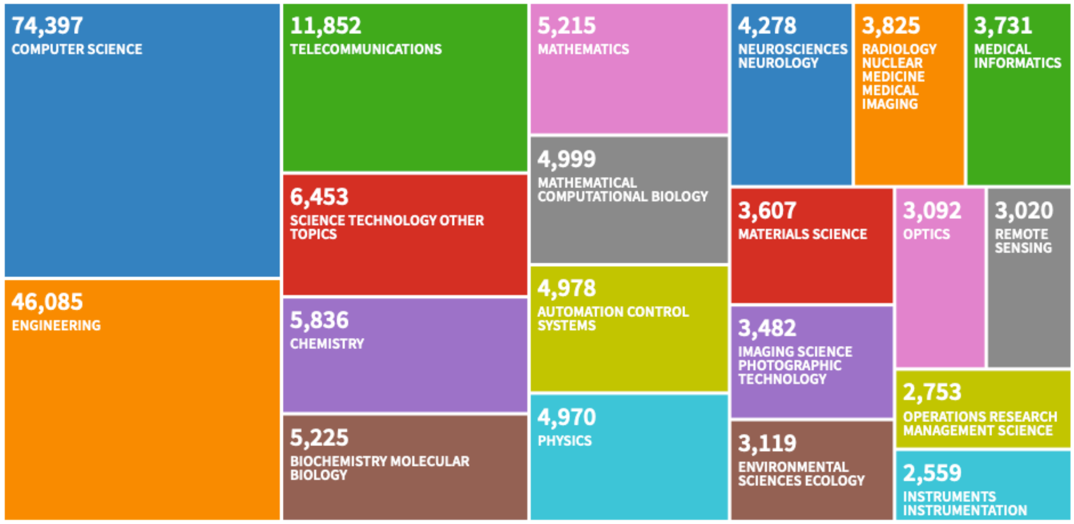


Figure 9: Machine learning research areas

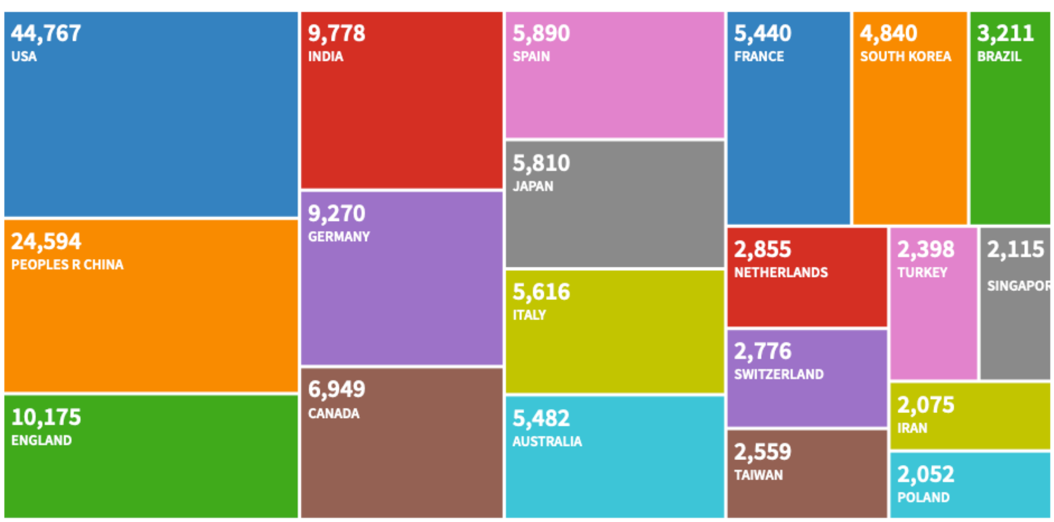


Figure 10: Machine learning research done in various countries and regions

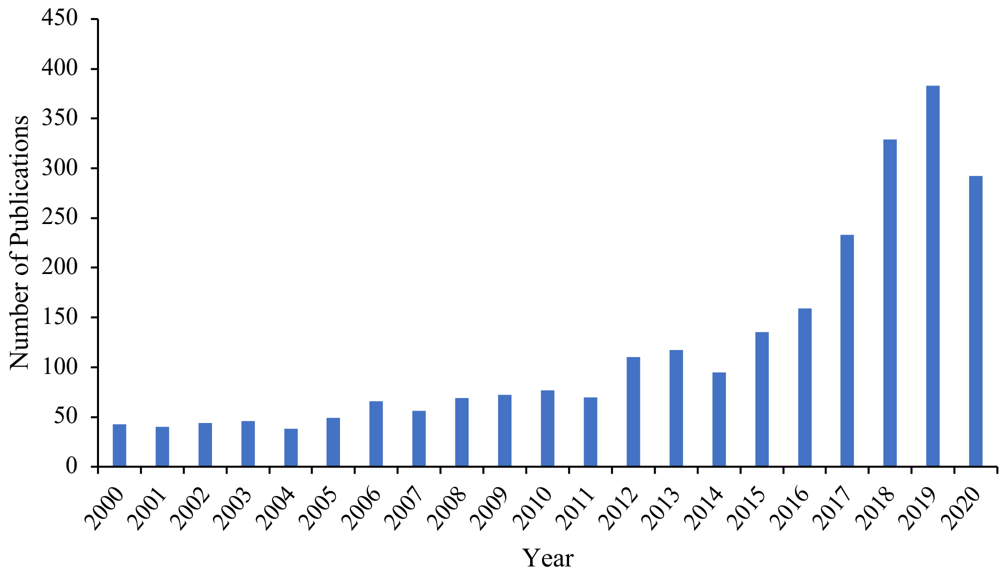


Figure 11: Predictive maintenance research publications over time

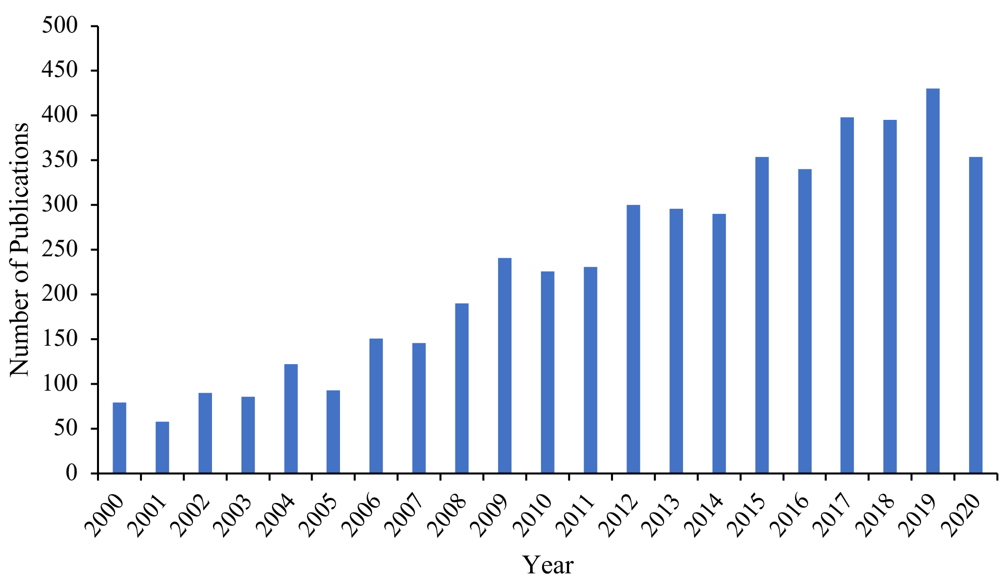


Figure 12: Preventive maintenance research publications over time

3.2. Data-Driven Modeling

Decision-making models for the planning, scheduling and control of maintenance can involve a number of different components which include: resource allocation, logical constraints, and cost quantification. However one component that is prevalent in all maintenance models to varying extents is failure modeling.

Accurate modeling of failure phenomena is challenging due to a high degree of intrinsic complexity, variability, and interaction. Nevertheless, two main approaches have emerged: (1) physics-based modeling, and (2) data-driven modeling. Physics-based modeling involves the use of first-principles constitutive equations to capture the dynamic behavior of material, energy, pressure, stress, and momentum within failure-prone systems. While one can formulate physics-based models for failure in principle and obtain accurate results using methods such as finite element analysis and computational fluid dynamics, in practice their implementation suffers from intractability. This stems from solving possibly stiff systems of differential-algebraic equations over fine grids leading to a large amount of computational time being required. Data-driven modeling on the other hand can obtain accurate results in less computational time and involves the use of data to construct surrogate models of the failure phenomena. Table 8 summarizes the related literature [9, 21, 27-127].

Table 8: Detailed indicative summary of data-driven failure modeling research

Inputs	condition data: vibration, acoustic, current, voltage, torque, power, displacement, temperature, thickness, chemical composition maintenance data: errors, failure and maintenance times process data: overload times , pressure fluctuations, flowrates, fuel-air-ratio, pumped volume, speed, concentrations, fuel consumption product data: quality, thickness environmental data: wind speed, humidity, air temperature, holidays
Methods	classification: logistic regression, naïve bayes, decision tree, random forest, support vector machine, one-class classification, neural networks regression: linear regression, auto regressive integrated moving average, Markov-chain Monte Carlo, gaussian process regression, decision tree, random forest, neural networks, self-organizing maps dimensionality reduction : principal components analysis clustering: k-means, k-nearest neighbors miscellaneous: physics-based extended Kalman filter, dynamic time warping, Bayesian networks
Outputs	discrete: failure occurrence, failure type, failure cause continuous: failure time, remaining useful life, failure probability, future condition, degradation rate
Fields	extractive: oil & gas, mining manufacturing: car, steel, semiconductors, chemicals power: wind, nuclear, transmission transportation: aviation, trucking miscellaneous: building, agriculture

The majority of research efforts have involved classification using individual models to determine whether or not failure would occur in a given time period. In other words, the output of the prediction is discrete. Prytz and coworkers [89] used vehicle air compressor operational data to determine whether a failure would occur before the next scheduled service visit. They performed feature selection using a beam search wrapper method as well as a Kolmogorov-Smirnov filter method, balancing using Synthetic Minority Over-sampling Technique (SMOTE), and classification using a random forest algorithm with an average accuracy of approximately 68%. They observed that automated feature selection yielded better results than feature selection by human experts. Zeng and coworkers [123] used support vector machine classification with simultaneous feature selection involving hyperparameter optimization using fuzzy adaptive particle swarm optimization to determine whether or not to do maintenance. They leveraged a large variety of rotating car manufacturing machinery data such as overload times, date of last maintenance, vibration, humidity and showed that support vector machine classification with an accuracy of 85% had a higher performance than logistic regression with an accuracy of 65%. Classification methods are not restricted to the manufacturing industry and for example Robles-Velasco and coworkers [94] demonstrated an application of logistic regression and support vector machine classification to a pipe network and predicted breakage in a year with a 75-80% accuracy and 73-87% recall.

Other efforts have involved regression to predict a continuous output. This has typically been done via the creation of data-driven parametric models such as linear regression models. An example of a parametric regression model is the Weibull model used in preventive maintenance which has been used to develop a two-parameter model of the failure probability distribution of equipment from time-to-failure data. Gebraeel and coworkers [50] used regression to determine the parameters of an exponential degradation signal model from vibration data to model the remaining useful life distribution of a bearing. Non-traditional regression models such as support vector regression in which the model structure and parameters are expressed more terms of data points also exist. Hong and coworkers [56] employ Gaussian process regression (GPR) and wavelet neural network models on bearing vibration data. They performed feature extraction to obtain the signal kurtosis as well as crest factor and select root mean squared (RMS) as the degradation indicator to predict. They showed that the Gaussian process regression model had a higher accuracy than the wavelet neural network model, and that both models had an error of 0.1% - 6.3% on their system.

Dimensionality reduction techniques have been employed extensively to perform fault detection, however for predictive maintenance these techniques have mainly been used as a feature extraction as well as feature selection pre-processing steps prior to using other methods for model creation. Baptista and coworkers [33] used principal components analysis as an intermediate step to generate new features for forecasting the time to fault using a variety of regression methods (support vector regression, random forest, generalized linear regression, neural networks) and unsupervised learning (k-nearest neighbors). Sun and coworkers [108] on the other hand used analysis of the principal components for selection of rolling element bearing vibration signal features to input into support vector machine regression. They then optimized the support vector machine hyperparameters with particle swarm optimization and obtained a model that had a 5% error on testing data.

Unsupervised learning techniques such as clustering have been employed for direct fault classification, however more often than not, they have been used for multi-class fault type classification to partition the data such that models can be built for each cluster. This has the advantage of improving model accuracy because models are customized to a narrower data distribution. Pinto and coworkers [87] used k-nearest neighbors and other methods for direct fault classification to determine which robots would break in a manufacturing context. Of interest is their use of specific load data such as the number of times robot arm rotated more than 200 degrees which gave an indication of overloading and extra stresses that could lead to enhanced degradation and premature failure. The results of their study were that the k-nearest neighbors had an accuracy of 98%, a precision of 98%, and a recall of 98%. Yang and coworkers [120] built clusters corresponding to different faults using ambient air and engine exhaust gas temperature via k-means clustering. They then constructed a different support vector machine regression model for each cluster to estimate the time to failure. This research was one example of different data-driven modeling paradigms being combined and in this case involved unsupervised learning and supervised learning to improve accuracy of future failure prediction.

Data-driven methods dominate the literature but a few but significant research efforts into the use of first-principles physics-based models exist. One such effort was carried out by Engeler and coworkers [47] who plugged measurements into first-principles equations to simulate condition variables of interest. Specifically, they performed parameter estimation by feeding online measurements of the current, torque, and position of a rotating manufacturing machine tool with a motor to determine the condition indicator of friction. This condition indicator was then used to label the equipment as being in a normal or degraded state based on whether was within exponentially weighted moving average (EWMA) control limits. However in practice such first-principles methods often requires the use of reduced order models such as the extended Kalman filter (EKF) employed by Wang and coworkers [121]. They used a state-space observer to determine whether or not to repair fuselage panels based on aircraft fuselage geometry measurements. They showed that the condition-based method was cheaper than scheduled or threshold-based maintenance.

Recently, ensemble methods have emerged as a way to improve the accuracy of predictions. A distinction is made here between individual models, which is used to denote standalone data-driven models, and ensemble models, which is used to denote a system of individual models. The underlying principle of ensemble models is to generate a prediction based upon some form of consensus. In other words, input data is fed to each individual model in the group, each of the individual models returns a prediction, and then some decision logic is employed to aggregate the individual predictions into a group prediction. In the context of binary classification, ensemble classification can take the form of simple majority voting in which each classifier is given one vote and the output of the ensemble classifier is the class with the most number of votes, or weighted majority voting in which each vote is weighted more or less according to some criteria. In the case of regression, the majority vote can be thought of as a simple or weighted arithmetic or geometric average of each of the individual regression model predictions. Nozari and coworkers [80] used an ensemble of classifiers consisting of random forest, support vector machine, partial-least squares, and naïve Bayes to determine the existence a fault on a simulated spacecraft. They observed that the ensemble of classifiers outperformed the individual classifiers. Pashazadeh and coworkers [85] reported an ensemble accuracy of 97% for their wind turbine application and employed an ensemble consisting of neural network, radial basis function, decision tree, and k-nearest neighbors classifiers. Gutschi and coworkers [53] extended the ensemble approach to construct multiple ensemble random forest classifiers that were each based on different sample horizons. They used this approach to predict the failure of milling machines with a prediction horizon of 168 hours with an average precision of up to 88%.

These data-driven models are then used to provide explicit prediction via parameters, or implicit predictions via equations in maintenance optimization models.

3.3. Maintenance Optimization

Maintenance optimization involves the development of models that assist with decision-making related to how to carry out maintenance activities on a set of assets subject to time and resource constraints. This decision-making is typically done in two overlapping but distinguishable approaches: (1) maintenance planning, in which time horizons span multiple months or years and decisions often relate to capacity, and (2) maintenance scheduling in which time horizons span multiple hours or weeks and decisions often relate to task allocation. Maintenance optimization methods seek to determine the sequence of maintenance actions that best minimizes the overall cost, maximizes the overall availability, and maximizes the overall effectiveness of performing maintenance. There are a variety of ways in which the optimization can be conceptualized and this has given rise to a large amount of research over the past three decades [2, 5-7, 128-225] spanning various aspects mapped out in Table 9.

Generally speaking, maintenance optimization can be further categorized along four major axes: (1) deterministic vs stochastic, in which approaches vary depending on the extent to which uncertainty in parameters is accounted for; (2) single objective vs multi-objective optimization, in which approaches consider either one objective function or consider tradeoffs; (3) mathematical vs metaheuristic optimization, in which approaches differ in rigor, optimality gap, and guarantee of optimality; and (4) perfect vs imperfect renewal, in which approaches differ in the extent to which maintenance reduces the effective age of equipment. Selected research in each of these axes is subsequently elucidated.

Table 9: Detailed indicative summary of maintenance optimization research

Planning	objective functions: long-term overall cost, availability, system effectiveness decision variables: manpower allocation, test intervals, maintenance cycles, inventory, maintenance type, maintenance policy, availability thresholds
Scheduling	objective functions: schedule cost, availability, system effectiveness, job tardiness, decision variables: manpower allocation, skill-type allocation, test intervals, maintenance cycles, task sequences, production rates, throughputs
Common Methods	age renewal: as-good-as-new, imperfect stochastic optimization: deterministic, chance-constrained, stochastic programming mathematical formulation: mixed-integer programming, mixed-integer linear programming, mixed-integer nonlinear programming, state-task network, Markov chain, fault tree, reverse fault tree metaheuristic optimization: genetic algorithm, particle swarm optimization, simulated annealing, reinforcement learning multi-objective optimization: none, lexicographic goal programming, epsilon-constrained
Fields	energy: wind, oil and gas manufacturing: job shop, batch, car, subtractive, semiconductor, chemicals, refining, air separation transportation: naval, rail, power miscellaneous: generic, buildings, farming, cloud computing

Deterministic maintenance optimization is seen to dominate the research space with fairly limited work done on stochastic maintenance optimization. As such two seminal works in stochastic maintenance optimization are provided and the subsequent other works described all involve deterministic optimization. Dedopoulos and Shah [145] used stochastic programming and mixed-integer linear programming to determine whether or not to perform maintenance on multipurpose equipment over the horizon. The uncertainty they considered at each time stage was equipment failure discretized into two scenarios: failure, or no failure. They formulated their system in state-task network representation and solved it via a multistage approach over a scheduling horizon of 1 week and a planning horizon of 5 years to obtain an optimal preventive maintenance plan that was periodic in nature. Duffuaa and Al-Sultan [149] also introduced a stochastic component to their maintenance model formulation by accounting for uncertainty in a task being required via consideration of the possibility of a job arriving with a certain probability. They used mixed-integer linear programming to determine the best way to allocate differently-skilled technicians to tasks and how much reserve manpower to keep on hand. They compared the stochastic maintenance optimization approach to the deterministic maintenance optimization approach and showed that value of the stochastic solution approach was a 10.6% reduction in maintenance cost.

The two seminal works also represent single-objective problems, however these approaches can be extended to multi-objective problems. Marseguerra and coworkers [174] simultaneously optimized system availability and variability of system availability using a genetic algorithm to determine an inspection interval sequence. Moghaddam and coworkers [179] used a data-driven Weibull model to capture system reliability and assist in determining an optimal preventive maintenance plan. They used a simulated annealing algorithm to determine the times at which to maintain and replace different components so as to simultaneously optimize cost and reliability.

Maintenance optimization has continued in recent years and has extended previous work to maintenance optimization integrated with design and/or production. Ye and coworkers [213] developed a mixed-integer nonlinear programming model and algorithm to solve a continuous-time Markov chain to decide which parallel units to install and their inspection intervals. This work represented simultaneous optimal system design and maintenance planning. Pan and coworkers [183] used mathematical programming to do integrated scheduling of production and maintenance so as to minimize the maximum job tardiness. They incorporated a condition-based data-driven multivariate linear regression degradation model to guide the optimization towards decisions that prevented degradation from exceeding user-specified degradation thresholds. Kopanos and coworkers [160] used a power consumption regression function in a resource-constrained mixed-integer linear programming scheduling model to minimize the cost running the compressors of an air separation plant. They considered operational decisions such as start-up, shutdown, and header assignment as well as maintenance decisions. They showed that using a flexible maintenance policy on their system with optimized non-periodic maintenance times led to a lower maintenance cost than a rigid maintenance policy with fixed maintenance times. Mathematical optimization methods have the benefits of being systematic and having a theoretically proven guarantee of optimality, however their use for extended multi-period problems for large complex systems can be challenging with large amounts of computational power potentially required to combat combinatorial explosion induced by all the possible combinations of binary variables despite algorithmic advances.

Metaheuristic optimization methods have shown promise in obtaining good feasible solutions to complex maintenance problems despite the absence of a theoretical guarantee of optimality. Amelian and coworkers [132] used a genetic algorithm in tandem with a particle swarm optimization algorithm to optimize the job sequence, production rate, and preventive maintenance time of a single-machine system. Wang and coworkers [205] leveraged recent advances in machine learning to obtain the optimized maintenance policy for a single generic machine using a semi-Markov model recast as a Q-P learning problem and solved it with a reinforcement learning algorithm. Yang and coworkers [211] used a genetic algorithm to obtain an optimized maintenance schedule for a manufacturing system of ten machines. They also compared corrective, scheduled, condition-based, and predictive maintenance approaches and showed that predictive maintenance had the highest net value. It can be noted that many metaheuristic methods are unconstrained optimization methods and as such do not have constraints naturally built into them. However maintenance and production optimization involves considerations relating to resource capacity, unit availability, mass balances, safety, and logical maintenance constraints. As such, the use of mathematical optimization methods lends itself more readily and naturally to planning and scheduling maintenance in higher fidelity through the use of equality and inequality constraints to capture these various maintenance considerations.

One such consideration is the maintenance imperfection, or the idea that the action of repairing equipment only restores equipment partially. The vast majority of literature including many of the works mentioned here assume maintenance to perfectly restore equipment to an as-good-as-new condition so as to help simplify the mathematical formulation and improve computational tractability. Sachdeva and coworkers' work [190] for instance leveraged the as-good-as-new assumption in using a genetic algorithm for multi-objective nonlinear programming to determine optimized preventive maintenance intervals. Their results showed that optimization resulted in a 1.3% increase in steady-state system availability, a 31% decrease in average maintenance time, and a 56% decrease in maintenance cost. Sanchez and coworkers [191] on the other hand considered maintenance as being imperfect. They compared two imperfect maintenance models: proportional age setback in which maintenance can reduce the entire age of the equipment by a fraction, and proportional age reduction in which maintenance can reduce the age the equipment gained only since the last maintenance by a fraction. They fed both models into a genetic algorithm to optimize test and maintenance intervals and showed that the proportional age setback model was slightly more conservative in describing unavailability but resulted in a lower maintenance cost than the proportional age reduction model. It is noted that this highlights the possibility of epistemic uncertainty in traditional maintenance models.

Parametric uncertainty in terms of the extent to which maintenance reduces the effective age of equipment can also observed. There is also significant amount of uncertainty in the parameters used in surrogate models in preventive maintenance research. This uncertainty stems from the data and methods used to construct these models. In practice the data used is solely time data, and is typically collected for a fleet of assets and/or for a single piece of equipment over a long time horizon. The challenge is that different assets in the fleet, and indeed a single piece of equipment over a long enough time, can experience different service conditions. This in effect ensemble-averages and time-averages the failure behavior of equipment. Maximum likelihood estimation is then done to estimate the parameters of the preventive maintenance surrogate models and these parameters are then stored in databases to aid decision-making. However it should be noted that these databases contain generic data from the viewpoint of application, and that they often do not take the state and context of individual equipment into account. This can result in practitioners often using this data in different services than originally measured. This can additionally result in assuming worst-case scenarios for numbers and excessive and costly conservatism. In other words, the parameters underlying the failure behavior of equipment are themselves time-dependent and condition-dependent distributions but are often treated as single-point deterministic values. This further motivates the use of data-driven models to enable accurate and customized failure and maintenance modeling with enough of the right data.

3.4. Process Control

Failure is an inherently dynamic process and process control represents another layer of protection for system resilience. Several related primarily model-based approaches existing in the literature [226-294] can be mapped out in Table 10.

One key underlying consideration is when to solve the control problem. This can be done in two ways: (1) online, via model predictive control; or (2) offline via explicit model predictive control. Model predictive control aims to optimize control actions in real time by using an embedded dynamical system model to predict the desired future evolution of the system at each time step. However model predictive control for large scale or nonlinear systems can suffer from computational challenges leading to slow latency [295]. Explicit model predictive control seeks to avoid this challenge by shifting the computational burden ahead of time instead. Multiparametric explicit model predictive control has emerged as a key research area [270] and offers a number of advantages such as: (1) the optimization problem is solved offline once; (2) obtaining of optimal control actions is reduced to rapid map-reading and function evaluation; (3) *a priori* possession of the full map of control solutions imparts additional knowledge for decision-making; and (4) having an explicit control solution enables integration with other levels of optimization without having to solve an embedded dynamic optimization problem.

Table 10: Detailed indicative summary of related process control research

Scope	**objective functions:** setpoint tracking, extent of input changes, constraint prioritization, disturbance rejection, average production rate **decision variable trajectories:** rotational speed, drug infusion rate, cooling, power, **single-unit systems:** reactors, batch bioreactors, tanks, distillation columns, air separation units, heat exchangers, simulated human patients, fuel cells, turbine **multi-unit systems:** coupled reactors, heat and power networks, solar fields, wind farm, **multi-level integration:** none, with scheduling, with design
Methods	**model reduction:** Kalman-type observer, system identification, autoregressive with extra input, data-driven regression, neural networks **state estimation:** model predictive control for moving horizon estimation, support vector machine, random forest, auto regressive integrated moving average, ensemble classification, ensemble regression **solution:** mixed integer linear programming, graph-based algorithms, reinforcement learning
Variants	**types:** proportional-integral-derivative, state-feedback, model predictive control, robust model predictive control, economic model predictive control, multiparametric model predictive control, data-driven regression, fault-tolerant control
Fields	**energy:** cogeneration, refining, wind, hydrogen, fuel cells **manufacturing:** chemical, pharmaceuticals, medicine **miscellaneous:** building ventilation

Other related considerations are subsequently elucidated: (1) model reduction, (2) state estimation, (3) fault-tolerant control; and (4) multi-level optimization.

The high-fidelity differential and algebraic equations used to accurately describe dynamical systems are often intractable for control applications which motivates of model reduction to obtain surrogate models. Georgiadis and coworkers [247] modeled a metal-hydride tank with a spiral heat exchanger from first principles and then used system identification to obtain an autoregressive with extra input surrogate process dynamical model. They then used the PARametric Optimisation and Control (PAROC) framework to obtain an optimal cooling flowrate profile to achieve high storage efficiency within a relatively short time. Katz and coworkers [252] explored the non-traditional use of machine learning for surrogate reduce-order model development in process control. They embedded a neural network with a rectified linear unit activation function within the control formulation by reformulation using mixed-integer linear programming and were able to control a bioreactor explicitly to maximize biomass concentration. Another interesting effort from the perspective of integrating a surrogate model for safety into process control was carried out by Albalawi and coworkers [226]. They used a safeness index based on normalized weighted magnitude of deviations from concentration and temperature setpoints, and used it to maximize average production rate.

State estimation methods represent an alternative to embedding the entire high fidelity model into the control formulation. While state estimators can themselves be embedded, state estimation is used here to denote standalone models that act as soft-sensors to models selected aspects of the high fidelity model behavior and thereby provide measurements of system outputs. Nașcu and Pistikopoulos [264] demonstrated an approach to solving the traditional state estimation problem by using multiparametric programming for moving horizon estimation. They estimated the anesthesia concentration within a simulated patient and optimized the trajectory of pumped anesthesia flowrate control actions. It was shown that the multiparametric moving horizon approach had better performance than Kalman estimators or traditional moving horizon estimation. Onel and coworkers [267] used time-specific random forest algorithms to estimate the magnitude of sensor and actuator faults after performing simultaneous fault detection and diagnosis using support vector machine classification. They then fed the estimates of the fault states into a multiparametric model predictive controller to manipulate water flowrate so as to control the temperature of a penicillin batch reactor.

It is noted that although data-driven methods are often used for model reduction and state estimation in conjugation with model predictive control, recent efforts have shown promise in using them to more deeply complement model predictive control. Reinforcement learning for instance is emerging as a way to overcome the computational challenges associated with solving online model predictive control models. Supervised learning has additionally been demonstrated to be able to approximate an entire model predictive controller as demonstrated by Shokry and coworkers [286]. They started by developing sets of input-output open loop data on states and their optimal control actions. They then created machine learning regression models to obtain explicit control laws. The models had a root mean squared error of less than 4%, took 77-99% less time.

One interface between maintenance and process control can be found in the field of fault-tolerant control. The objective of fault-tolerant control is to obtain optimized trajectories of control actions that are able to reject process disturbances induced by faults while maintaining system performance and closed loop stability. Bernardi and coworkers [232] considered actuator faults as inducing a process disturbance and use model predictive control for fault-tolerant control. They developed a state-space model for a heat exchanger and for a CSTR via the parameterized Jacobian linearized technique and estimated fault magnitude using a reduced-order observer. They observed for their application that in the presence of faults, non-fault-tolerant model predictive control was not able to achieve desired setpoint tracking in contrast with fault-tolerant model predictive control. Kettunen and coworkers [254] explored three methods of introducing sensor fault tolerance into control: (1) replacing the measurement entirely, (2) correcting the measurement slightly, and (3) correcting the reference trajectory. They did fault detection using principal components analysis, partial least squares, and subspace identification together with an alarm policy. They then compared the use of proportional-integral control and model predictive control for a heavy oil fractionator process and showed that model predictive control had a better performance than model predictive control. Chillin and coworkers [239] investigated the control of a benzene catalytic alkylation process with the aid of fault magnitude estimation using a parameter estimation approach. They observed that fault-tolerant control led to fewer wasted control actions than with non-fault-tolerant control and was cheaper.

Another pertinent aspect of process control in this space is its demonstrated potential for integration with other levels of optimization such as scheduling and planning. Baldea and Harjunkoski [230] described the integrated scheduling and control problem and demonstrated it with a multi-product CSTR scheduling example. They also introduced the concepts of time-scale bridging, and distinguished between sequential and simultaneous approaches to tackling the integrated scheduling and control problem. This was followed by work on reducing computational time through the integration of scheduling and explicit multiparametric model predictive control by Burnak and coworkers [237]. They used a high fidelity multi-product CSTR model together with the PAROC framework to obtain a piecewise affine function for the optimal control actions depicted as a control map. They then leveraged a surrogate time-scale bridging model to incorporate the optimal control actions into an multiparametric mixed integer quadratic programming scheduling model for two CSTR's in parallel. In effect their work can be conceptualized as follows: (1) a control-aware scheduling model providing optimal setpoints to a scheduling-aware control model, and (2) that scheduling-aware control model determining the optimal way to transition between scheduled continuous setpoints. Process control can also be integrated with design as shown by Diangelakis and coworkers [241] who obtained the optimal designs and control schemes for a tank, CSTR, distillation column, as well as a combined heat and power network. They demonstrated a proof of concept for solving challenging integrated design-control problems with this approach and simultaneously obtained closed loop stability and cost optimal designs.

3.5. Process Safety Quantification

Maintenance directly affects the level of safety present in productive processes. This is due to the fact that when it is absent, the levels of degradation of process equipment are allowed to increase unchecked leading to failures of process units. These failures of process units can engender domino effects of events that can lead to catastrophic consequences. Of note is that the way that the process is operated can also help avoid process incidents. As such there has been great interest in the literature in developing numerical methods to quantify the level of safety so as to increase it by changing process and maintenance variables [12, 295-339]. Selected approaches have been provided in Table 11 in lieu of a detailed exposition.

The currently accepted gold standard in the process safety community is the use of Bayesian networks for process safety quantification. Adedigba and coworkers [297] investigated the dynamic failure analysis of a crude oil distillation unit by combining a fault tree for barriers and event tree for consequences into a Bayesian network to predict system probability of failure. It is however noted that use of Bayesian networks in optimization is challenging due to their mathematical complexity leading to slow computational times. This motivates the development of process safety metrics simple enough to be used for maintenance optimization with mathematically complex dynamical system aspects described by data-driven models.

This chapter covered a variety of different aspects. The identified research gaps were provided in the introduction. This concludes the literature review.

Table 11: Overview of dynamic process safety quantification research

Reference	Approach
[226]	Safeness Index (ASI)
[299]	Dynamic Bayesian Network
[301]	Bayesian Network
[302]	Risk index (CRI)
[303]	Safety Resilience Index (SRI)
[304]	Dynamic Fault Tree
[306]	Stochastic Hybrid Fault Tree Automaton (SHyFTA)
[307]	System dynamics causal graph and HAZOP
[340]	Functional Resonance Analysis Method (FRAM)
[311]	Process Resilience Analysis Framework (PRAF)
[312]	Fuzzy dynamic fault tree
[313]	Event tree analysis with Bayesian probability updating
[314]	Dynamic Bayesian Network
[316]	Quantitative Bow-tie Analysis
[317]	Integrated inherent safety index (I2SI)
[318]	Safety Weighted Hazard Index (SWeHI)
[323]	PROCedure for the Evaluation of Operational Safety
[324]	Real-time probabilistic risk analysis
[325]	Dynamic Bayesian Network
[328]	Dynamic procedure for atypical scenarios identification
[330]	Quantitative Index of Inherently Safer Design (QI2SD)
[331]	Event Sequence Diagram
[195]	Flexibility-reliability-criticality index (FRC)
[332]	Domino Hazard Index (DHI)
[336]	Dynamic operational risk assessment (DORA)
[334]	Hierarchical Bayesian Approach (HBA)

4. DATA-DRIVEN PREVENTIVE MAINTENANCE PLANNING

4.1. Summary

Maintenance is an essential part of mechanical integrity programs and aims to prevent the occurrence of process safety incidents and costly unplanned shutdowns. Maintenance can increase the availability of equipment in productive systems and effective preventive maintenance programs enable maintenance activities to be planned proactively. However, maintenance planning is subject to resource scarcity and is rendered nontrivial due to system complexity, reliability model nonlinearity, and parametric uncertainty. Multi-objective stochastic mixed-integer nonlinear programming is well suited to addressing these challenges and is adopted here to optimize when to perform maintenance on different pieces of equipment.

A model is formulated and optimized accounting for: the effect of imperfect repair using an effective age model, equipment failure behavior using a data-driven Weibull reliability model, endogenous uncertainty in reliability model parameters, and the simultaneous need to satisfy the competing objectives of cost minimization and reliability maximization. The results of the research consist of optimal maintenance plans, plots of resultant equipment and system reliability over time, and a frontier of optimal solutions from which the decision maker can select. The approach adopted here is illustrated with two case studies and can be extended to improving the overall availability, effectiveness, and resilience of a variety of productive systems.

4.2. Introduction

Maintenance refers to activities designed to improve system resilience and system availability and avoid the failure of system components. Unplanned system shutdowns and slowdowns due to failed system components can be costly and result in significant losses in productive capacity due to downtime. Crucially however, the reduction of system resilience due to ineffective maintenance can lead to catastrophic process safety incidents such as the Texas City refinery incident in which there were 15 fatalities, 180 injuries, and over $1.5 billion in financial losses [341]. The allocation of finite resources in complex systems to improve system resilience often exhibits diminishing marginal returns and is further complicated by the presence of parametric uncertainty. This research contributes to meeting this challenge and presents a systematic approach to address the multi-objective and stochastic nature of maintenance planning using optimization.

Maintenance encapsulates a plurality of technical and socio-organizational concepts. As used here, maintenance activities refer to proximate acts undertaken to improve the availability of system components and thereby increase the availability of ageing productive systems. These activities may include monitoring, inspection, cleaning, lubrication, testing, repair, or replacement depending on requirements. Maintenance can help to improve mechanical integrity, aid in preventing process safety incidents, and avoid costly downtime due to unplanned shutdowns and slowdowns. Maintenance involves optimal resource allocation and the decisions of when, where and how to do maintenance are key.

Commonly adopted maintenance policies in industry include: (i) basing decisions on mean time to failure (MTTF) recommendations from original equipment manufacturers (OEM), (ii) scheduling maintenance at fixed intervals based on internal company data, (iii) corrective maintenance in which selected equipment are run to failure, (iv) condition-based monitoring and predictive maintenance, (v) risk-based inspection, and (vi) reliability-centered preventive maintenance.

Selection of the appropriate maintenance policy is in part informed by data availability, company culture, and the level of expertise available to create and provide support for developed solutions. It is noted here that the time horizon over which maintenance decisions are made influences maintenance policy selection. Planning is used here to denote high-level decisions taken over months or years and is distinguished from scheduling in which decisions are taken over hours, days, and weeks.

Equipment	**Y1**		**Y2**		**Y3**		**Y4**		**Y5**	
V-001		T		T		T		T		T
V-002	T		R		T		T		R	
⋮										
P-27	T	T	T	T	T	R	T	T	T	T
⋮										
C-11	T		T		R		T		T	

Figure 13: Generic maintenance plan

This research deals with optimal maintenance planning in which high-level discrete and continuous decisions are made in the absence of detailed information over relatively over long time horizons using a time discretization on the order of months or years. This is distinct from maintenance scheduling in which lower-level decisions are taken over shorter time scales on the order of weeks or days. A generic example of a maintenance plan is provided in Figure 13 in which different equipment are tested (T) and replaced (R) over a five-year planning horizon. Regardless of the maintenance policy selected, certain factors affect optimal resource allocation:

1. Company resources are limited and need to be carefully allocated among operations; business improvement projects; and health, safety and environmental (HSE) projects. The portion of the budget allocated to maintenance is consequently finite and must be decided *a priori*.

2. There are monetary costs associated with maintenance actions and increasing maintenance expenditure leads to diminishing marginal gains in reliability. In other words, the objectives of minimizing cost and maximizing reliability are conflicting and maintenance planning is multi-objective in nature.

3. Maintenance actions may be imperfect and do not necessarily restore equipment to either an 'as good as new' or an 'as bad as old' condition.

4. The functions used to rigorously estimate equipment and system reliability are nonlinear and their parameters are not known with absolute certainty.

A selected subset of related literature was provided in the preceding chapter. The objective of this research is to extend the previous efforts in the area by simultaneously considering imperfect maintenance, nonlinear reliability modeling, stochastic optimization, and multi-objective optimization. To this end: (1) the Weibull distribution is used to more accurately and consistently model the component reliability; (2) maximum likelihood estimation is used to rigorously estimate the imperfect maintenance factor, the Weibull scale parameter, and the Weibull shape parameter; and (3) uncertainties in the parameter estimates are considered and addressed using stochastic programming. The resulting model is a constrained stochastic multi-period mixed-integer nonlinear programming (MINLP) model. The objectives considered here are cost minimization and reliability maximization. The key decision variables include: the expected number of repairs, the expected number of replacements, whether or not to do maintenance in a time interval, and the sequence of maintenance actions over the time horizon.

The result of this research is a general framework for multi-objective stochastic preventive maintenance planning which can be used as a tool to determine plots of equipment and system reliability over time, the expected maintenance budget, the number of spare parts to keep in inventory, and a front of optimal maintenance plans corresponding to different system reliability thresholds.

4.3. Methodology

The maintenance model used here is data-driven and as such the first step of the methodology is estimating the reliability model parameters and their uncertainties. This can be done by obtaining equipment failure data and doing maximum likelihood estimation (MLE), or by expert judgement. Here the reliability model parameters are treated as an known inputs.

Following estimation of the reliability model parameters, the optimization model is formulated. The model is a multi-period multi-objective stochastic mixed-integer nonlinear mathematical programming model. This model is then optimized to obtain a maintenance plan. It is noted that McCormick relaxations and piece-wise linear approximations can be employed to help address nonlinearities. The model was implemented on two case studies.

4.4. Results

4.4.1. Case Study 1

4.4.1.1. Description

The system considered for the first case study consists of three identical centrifugal pumps in series shown in Figure 14. Case study parameters are shown in Table 12.

An assumption is made in this case study that repair maintenance actions extend the life of equipment by directly increasing the nominal value of the Weibull scale parameter (τ_0).as shown in Figure 15.

Table 12: Case Study 1 – Maintenance planning model parameters

Parameter	**Symbol**	**Value**
Equipment age lower bound, yr	age^{L}	0
Equipment age upper bound, yr	age^{U}	5
Time interval, yr	t_d	0.5
Scale parameter scenarios, yr	$\tau(\zeta)$	2.6, 3.0, 3.4
Scale parameter upper bound, yr	τ^{U}	3.6
Number of replacements upper bound	n_{spares}^{U}	10
Number of repairs upper bound	$n_{repairs}^{U}$	10
Normalized cost per repair	C_k	1
Normalized cost per replacement	c_{spares}	10
System reliability thresholds	$\widetilde{R_e}$	0.9, 0.95, 0.99, 0.995, 0.999
Imperfect maintenance factors	α_k	1, 0.1, 0
Shape parameter	$\beta(i)$	1.5, 1.5, 1.5

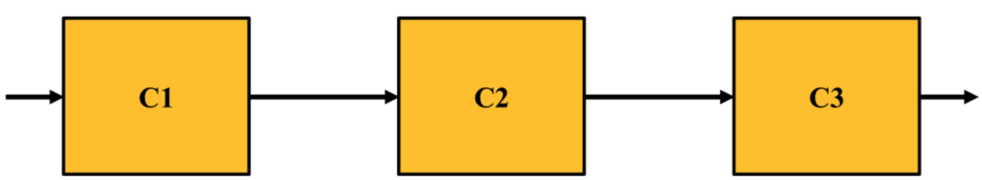


Figure 14: Pump system

It is further taken that the scale parameter is uncertain and assumed that this uncertainty follows a triangular probability distribution discretized into three scenarios. The triangular probability distribution is characterized by a minimum (a), maximum (b), as well as a nominal value (c) and was selected due to the relative ease of soliciting the parameter values from industry maintenance experts. It can thus be seen that under these assumptions, a repair maintenance action that would shift the nominal scale parameter from c_1 to c_2. This has the effect here of skewing the distribution and increasing the probability of realization of scenarios with a higher scale parameter value. It is noted that this represents endogenous uncertainty.

The probability distribution of the scale parameter under the assumptions was computed for different numbers of repair actions and then regressed as shown in Figure 16. These models were then implemented in the model formulation.

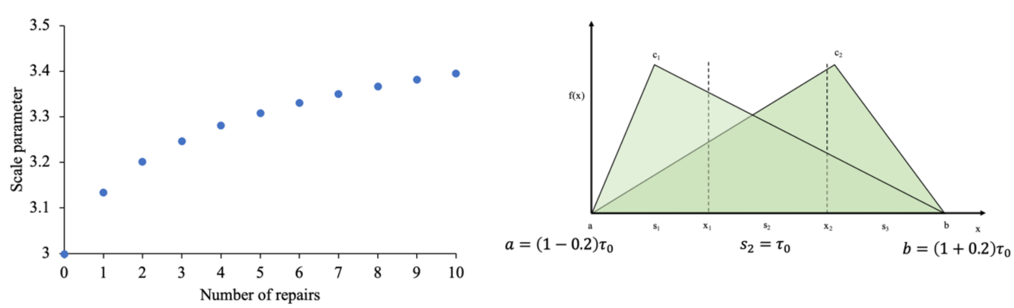


Figure 15: Case Study 1 - The modeled effect of repairs

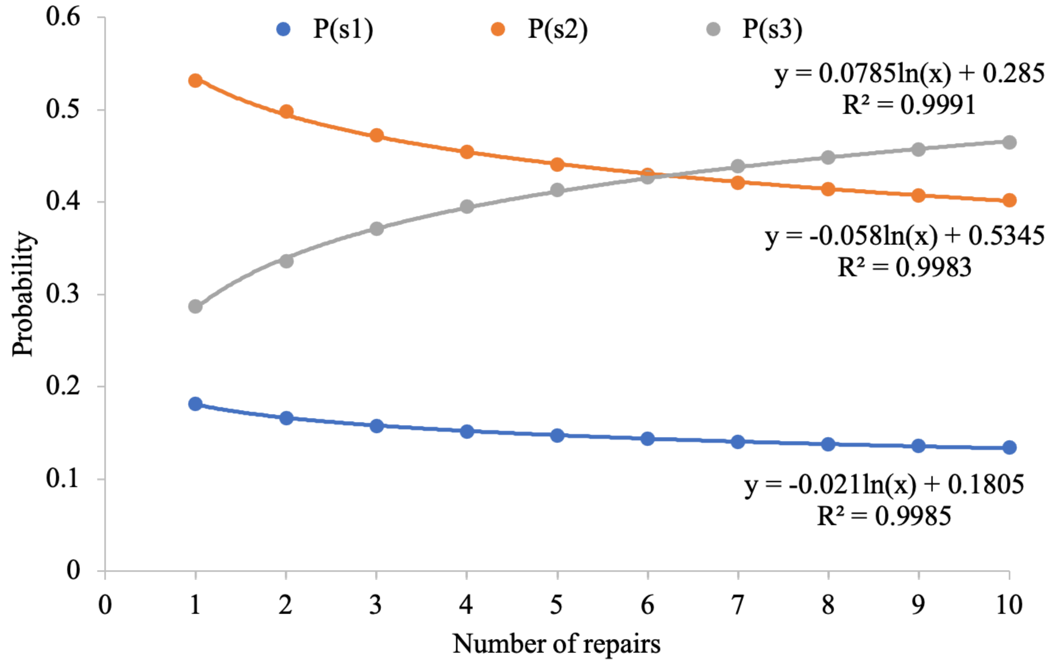


Figure 16: Case Study 1 - The modeled effect of the number of repairs

4.4.1.2. Model Formulation

Equipment are indexed by $i = 1, 2, \ldots, I$. Maintenance actions are indexed by $k = 1, 2, \ldots, K$, where k_1 is used to denote the absence of a maintenance action, k_2 is used to denote repair, and k_3 is used to denote replacement. Time intervals are indexed by $t = 1, 2, \ldots, T$ and scenarios by $\zeta \in Z$.

The decision variables used in the model are the Weibull scale parameter, τ, the effective age, age, the number replacements, n_{spares}, the number of repairs, $n_{repairs}$, and whether or not to perform a maintenance action in a time interval, m.

The first objective, is minimization of cost, J_1. The cost considered here is a function of the maintenance actions, and is parameterized by the cost coefficients C_k and c_{spares}. The second objective is the implicit maximization of system reliability, R_{sys}. The multi-objective method used here is smilar to the ε-constraint method with predefined reliability thresholds, $\widetilde{R}(e)$ where $e = 1,2,\dots,\xi$. A logarithmic transformation has been used here on system reliability and the system reliability thresholds to reduce nonlinearity. It is noted as that the resultant constraint on system reliability is linear and convex. These objectives are optimized subject to scalar and vector equality and inequality constraints.

$$\min J_1 = \sum_{i}^{I}\sum_{k}^{K}\sum_{t}^{T} C_k m(i,k,t) + \sum_{i}^{I}\sum_{t}^{T} c_{spares} m(i,k_3,t) \tag{3}$$

$$\ln R_{sys}(t) \geq \ln \widetilde{R}(e) \qquad \forall\, t \in T, e \in \xi \tag{4}$$

The execution of at most one type of maintenance action in each time interval is enforced by (5). The expected cumulative number of repairs and replacements performed over the time horizon respectively is determined by (6) and (7).

$$\sum_{k}^{K} m(i,k,t) \leq 1 \qquad \forall\, i \in I, t \in T \tag{5}$$

$$n_{repairs}(i,t) = \sum_{t'}^{t} m(i,k_2,t') \qquad \forall\, i \in I, t \in T \tag{6}$$

$$n_{spares}(i) = \sum_{t}^{T} m(i,k_3,t) \qquad \forall\, i \in I \tag{7}$$

An effective age model is used to capture the effect of the different maintenance actions on equipment condition as shown in (8) and (9). This is done through a nonconvex bilinear-integer-continuous (BIC) term that introduces an imperfect maintenance factor, α_k that scales the age increase. It can be seen that given a time discretization (t_d), the increase in effective age is equivalent to the increase in actual age when there is either no maintenance or it is as-bad-as old ($\alpha_k = 1$).

$$\mathrm{age}(i,t) = [\mathrm{age}(i,t-1) + t_d] - \sum_{k}^{K} \mathrm{BIC}(i,k,t) \qquad \forall\, i \in I,\ t \in T \tag{8}$$

$$\mathrm{BIC}(i,k,t) = m(i,k,t)(1 - \alpha_k)[\mathrm{age}(i,t-1) + t_d] \qquad \forall\, i \in I,\ k \in K, t \in T \tag{9}$$

Constraint (9) is replaced by a set of constraints for tractability.

$$m(i,k,t)\mathrm{age}^L \leq \mathrm{BIC}(i,k,t) \qquad \forall\, i \in I,\ k \in K, t \in T \tag{10}$$

$$\mathrm{BIC}(i,k,t) \leq m(i,k,t)\mathrm{age}^U \qquad \forall\, i \in I,\ k \in K, t \in T \qquad \forall\, i \in I,\ k \in K, t \in T \tag{11}$$

$$[(1-\alpha_k)(\mathrm{age}(i,t) + t_d)] - \big(1 - m(i,k,t)\big)\mathrm{age}^U \leq \mathrm{BIC}(i,k,t) \qquad \forall\, i \in I,\ k \in K, t \in T \tag{12}$$

$$\mathrm{BIC}(i,k,t) \leq [(1-\alpha_k)(\mathrm{age}(i,t) + t_d)] - \big(1 - m(i,k,t)\big)\mathrm{age}^L \qquad \forall\, i \in I,\ k \in K, t \in T \tag{13}$$

The scale parameter distribution is determined via (14) as previously described, and then used to calculate an effective scale parameter in (15). This then allows for the components and system reliability to be defined by (16) and (17) respectively.

$$p(\zeta, t) = f(n_{repairs}(i, t)) \qquad \forall\ i \in I, t \in T \qquad (14)$$

$$\tau_E(i, t) = \sum_{\zeta}^{Z} p(\zeta, t)\tau(\zeta) \qquad \forall\ i \in I, t \in T, \zeta \in Z \quad (15)$$

$$\ln\big(R(i, t)\big) = \left(\frac{1}{\tau_E(i)^{\beta(i)}}\right) age(i, t)^{\beta(i)} \qquad \forall\ i \in I, t \in T \qquad (16)$$

$$\ln R_{sys}(t) = \sum_{i}^{I} \ln R(i, t) \qquad \forall\ t \in T \qquad (17)$$

The model formulation is completed by a set of constraints that bound the variables.

$$age^L \leq age(i, t) \leq age^U \qquad \forall\ i \in I, t \in T \qquad (18)$$

$$0 \leq \tau_E(i) \leq \tau^U \qquad \forall\ i \in I \qquad (19)$$

$$n_{spares}(i) \leq n_{spares}^U \qquad \forall\ i \in I \qquad (20)$$

$$n_{repairs}(i) \leq n_{repairs}^U \qquad \forall\ i \in I \qquad (21)$$

$$m(i, k, t) = \{0,1\} \qquad \forall\ i \in I,\ k \in K, t \in T \qquad (22)$$

It is noted that formulated model represents a theoretical system. It can however be modified for use with series-parallel and other system configurations.

4.4.1.3. Maintenance Planning

Two sets of preliminary optimization results are provided here. The results consist of maintenance plans showing the optimal sequence of repairs (I) and replacements (P), plots of the corresponding equipment and system reliability against time, and a sensitivity analysis in the form of a curve showing different maintenance plans.

The first set of results corresponds to a maintenance policy in which a recommendation of a manufacturer to repair equipment once every three years is followed. The maintenance plan corresponding to this policy is shown in Table 13. It was observed that this policy rendered the model infeasible until the system reliability thresholds (J2) were relaxed. In less mathematical terms, this maintenance policy was inconsistent with the goal of maintaining system reliability above set thresholds over the entire time horizon. This is visualized in Figure 17, from which it can be observed that the equipment and system reliability profiles are below 90%, and by extension 99.5%, over the majority of the time horizon.

The second set of results corresponds to maintenance performed according to the methodology presented in this paper. The maintenance plan corresponding to a system reliability threshold of 99.5% is presented in Table 14. The equipment and system reliability profiles are visualized in Figure 18 and system reliability is seen to be maintained above the set threshold over the entire time horizon.

Table 13: Maintenance plan based on a manufacturer recommendation

Equipment	**n_{spares}**	**Y1**		**Y2**		**Y3**		**Y4**		**Y5**	
C1	0					I					
C2	0						I				
C3	0						I				

Table 14: Maintenance plan based on present methodology

Equipment	**n_{spares}**	**Y1**		**Y2**		**Y3**		**Y4**		**Y5**	
C1	5	P	I	I	I	I	P	P	P	I	P
C2	4	I	I	P	P	P	I	I	I	P	I
C3	1	I	P	I	I	I	I	I	I	I	I

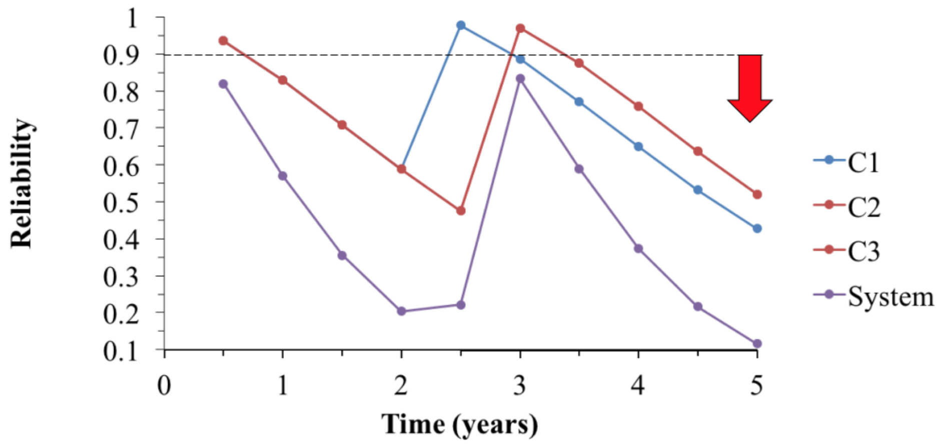


Figure 17: Reliability plot based on a manufacturer recommendation

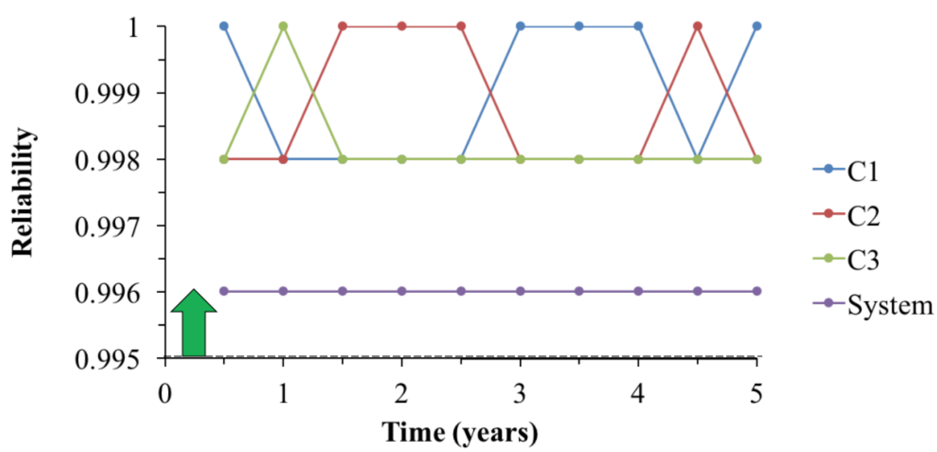


Figure 18: Reliability plot based on the present methodology

The results are dependent on the parameters used. The effect of changing the system reliability threshold is shown in Figure 19 in which each point corresponds to a different optimal maintenance plan and a trade-off between cost and reliability is observed.

It is noted that the curvature of the plotted set of solutions is a characteristic of the reliability thresholds used.

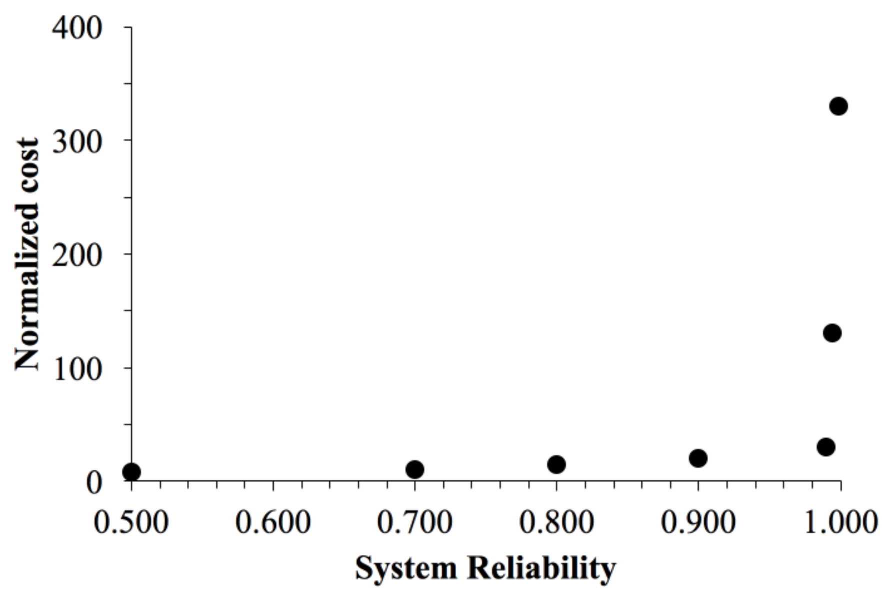


Figure 19: Case Study 1 - Optimal maintenance plans

4.4.2. Case Study 2

4.4.2.1. Description

The system considered for the second case study consists of a complex series-parallel arrangement of equipment used as part of an offshore cooling water system. The system is shown in Figure 20 and its corresponding parameters are provided in Table 15.

The function of the system is to reliably provide cooling water for downstream units. This is done using ten components $i \in I$ which consist of centrifugal pumps $(i1, i2)$, check valves $(i3, i4)$, isolation valves $(i5, i6, i7, i9)$, an automated control valve (i8), and a manual control valve $(i10)$. The components can be seen to belong to four subsets $P1 = i1, i3, i5$, $P2 = i2, i4, i6$, $A = i7, i8, i9$, and $M = i10$ that correspond to different subsystems. It is noted in passing that this system exhibits redundancy which is desirable from a reliability perspective.

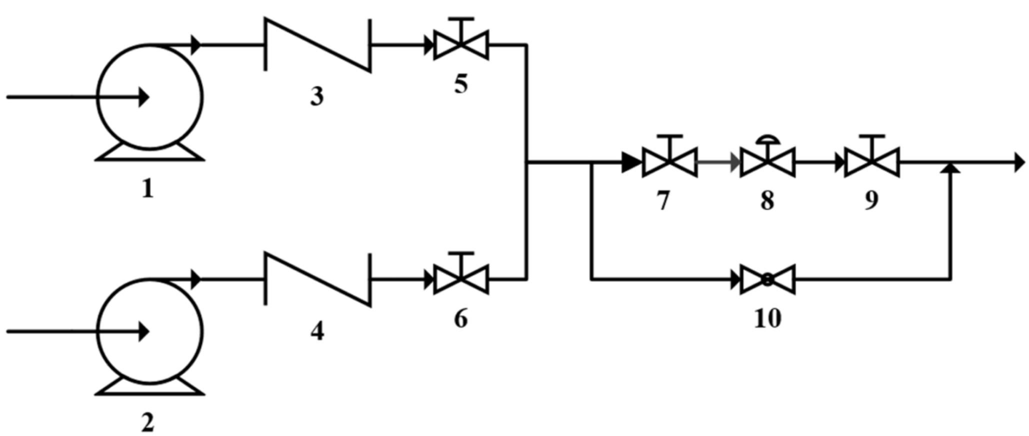


Figure 20: Case Study 2 - Offshore cooling water system

The focus of the second case study is on exploring the uncertainty of the imperfect maintenance factor. The imperfect maintenance factor is taken to be a given stochastic parameter that follows a discrete distribution with fixed realization probabilities. This corresponds to capturing uncertainty in the extent to which component degradation can be reversed.

It is noted that the approach to maintenance modeling in the second case study differs markedly from the first case study. Here, maintenance actions are not assumed to affect the reliability model parameters. The directionality of the imperfect maintenance factor is also different in that that a value of one corresponds to restoration to an as-good-as -new condition.

The maintenance planning horizon is three years with a time discretization of three months. The key maintenance actions considered here are repair and replacement. The absence of maintenance actions is an implicit additional action. The set of components that undergo repair is restricted to components i1, i2, i8, and i10 with the reliability of the other components taken as known time-varying parameters.

This case study was selected to illustrate the power of the approach on a more complex system. The system exhibits: (1) nonlinearity, due to the Weibull reliability model being an exponential function, (2) non-convexity, due to the power term in its exponent, and (3) component interactions, which are present in the system reliability function which is characterized by a 4th order polynomial.

Table 15: Case Study 2 – Maintenance planning model parameters

Parameter	Symbol	Value(s)
Equipment age lower bound, yr	$\mathrm{age}^{\mathrm{L}}$	0
Equipment age upper bound, yr	$\mathrm{age}^{\mathrm{U}}$	3
Time interval, yr	$\mathrm{t_d}$	0.25
Imperfect maintenance factor for inspection	$\alpha_{\mathrm{i,1,s}}$	0
Imperfect maintenance factor for testing	$\alpha_{\mathrm{i,2,s}}$	0
Imperfect maintenance factor for pump repair	$\alpha_{\mathrm{i,3,s}}$	[0.8, 0.9, 0.95]
Imperfect maintenance factor for repair of other components	$\alpha_{\mathrm{i,3,s}}$	0.9
Imperfect maintenance factor for replacement	$\alpha_{\mathrm{i,4,s}}$	1
Imperfect maintenance factor for doing nothing	$\alpha_{\mathrm{i,5,s}}$	0
System reliability thresholds	$\widetilde{\mathrm{R}}_e$	[0.5, 0.6, 0.7, 0.8, 0.9]
Maintenance cost, $	c_{k}	[50, 200, 1000, 1500, 0]
Component procurement cost, $	ϕ_{i}	[2380, 2380, 249, 249, 309, 309, 309, 1429, 309, 548]
Scenario probabilities	p_s	[0.3, 0.5, 0.2]
Time interval duration, yr	δ	0.25
Shape parameter	$\beta(\mathrm{i})$	[2.12, 2.12, 1.44, 1.44, 1.05, 1.05, 1.05, 1.35, 1.05, 1.1]
Scale parameter, yr	$\gamma(\mathrm{i})$	[1.14, 1.13, 349.32, 349.32, 12.86, 12.86, i7 12.86, 11.8, 12.86, 2.64]

4.4.2.2. Model Formulation

The model formulation involves components $i \in I$, scenarios $s \in S$, maintenance actions $k \in K$, and reliability thresholds $e \in E$.

The major decisions that the planning model seeks to inform are dived into two: (1) the first-stage here-and-now decisions of how many spares to procure ahead of time to keep on hand; and (2) the second-stage wait-and-see decisions of repair and replacement maintenance actions.

The first objective function considered is overall expected cost (J_1). This is divided into here-and-now procurement cost (Z^1) and a wait-and-see cost (Z^2) that is informed by maintenance actions ($m_{i,k,t,s}$) performed in the scenarios.

$$\min J_1 = Z_1 + Z_2 \tag{23}$$

$$Z^1 = \sum_{i \in I} \phi_i \, n_{i,k4} \tag{24}$$

$$Z^2 = \sum_{s \in S} p_s \sum_{i \in I} \sum_{k \in K} \sum_{t \in T} c_k m_{i,k,t,s} \tag{25}$$

The second objective function is system reliability ($R^{sys}_{t,s}$). It is noted that a conservative stochastic optimization approach has been employed here in which the reliability of the system is constrained to be above a threshold in every scenario.

$$R^{sys}_{t,s} \geq \widetilde{R}_e \qquad \forall t \in T, \forall s \in S \tag{26}$$

The cost and reliability are subject to a set of constraints that relate to the usage of resources, effective age, component reliability and subsystem reliability. The cost is dictated by the maintenance actions. The maintenance actions affect the effective age increase ($\Delta_{i,t,s}$) which affects the age of the components ($\tau_{i,t,s}$). This in turn affects component reliability ($R_{i,t,s}$) and system reliability.

Replacement is constrained to not be able to occur if no components have been procured by (27). It is noted that this is a linking constraint from a stochastic optimization perspective. The effective component age resulting from maintenance actions is defined by (28) and (29). In the case of replacement, the component age is reset by (30). Variable bounds are omitted for brevity.

$$m_{i,k,t,s} \leq n_{i,k4} \qquad \forall i \in I,\, k = 4,\, \forall t \in T,\, \forall s \in S \quad (27)$$

$$\tau_{i,t,s} = \tau_{i,t-1,s} + \delta - \Delta_{i,t,s} \qquad \forall i \in I,\, \forall t \in T,\, \forall s \in S \quad (28)$$

$$\Delta_{i,t,s} = \sum_{k \in K} \alpha_{i,k,s} \delta m_{i,k,t,s} \qquad \forall i \in I,\, \forall t \in T,\, \forall s \in S \quad (29)$$

$$0 \leq \tau_{i,t,s} \leq \left(1 - m_{i,k4,t,s}\right) age^{U} \qquad \forall i \in I,\, \forall t \in T,\, \forall s \in S \quad (30)$$

The component and subsystem reliability are then defined and used to compute the system reliability.

$$R_{i,t,s} = e^{-\left(\frac{\tau_{i,t,s}}{\gamma_i}\right)^{\beta_i}} \qquad \forall i \in I, \forall t \in T, \forall s \in S \quad (31)$$

$$R_{t,s}^{P1} = \prod_{i \in I^{P1}} R_{i,t,s} \qquad \forall t \in T, \forall s \in S \quad (32)$$

$$R_{t,s}^{P2} = \prod_{i \in I^{P2}} R_{i,t,s} \qquad \forall t \in T, \forall s \in S \quad (33)$$

$$R_{t,s}^{A} = \prod_{i \in I^{A}} R_{i,t,s} \qquad \forall t \in T, \forall s \in S \quad (34)$$

$$R_{t,s}^{M} = \prod_{i \in I^{M}} R_{i,t,s} \qquad \forall t \in T, \forall s \in S \quad (35)$$

$$R_{t,s}^{sys} = \left(R_{t,s}^{P1} + R_{t,s}^{P2} - R_{t,s}^{P1}R_{t,s}^{P2}\right)\left(R_{t,s}^{A} + R_{t,s}^{M} - R_{t,s}^{A}R_{t,s}^{M}\right) \qquad \forall t \in T, \forall s \in S \quad (36)$$

It is noted that three implementation strategies were employed to help reduce computational intractability. These were (1) bounding variables, (2) introducing McCormick envelopes successively for bilinear terms to obtain a mixed-integer linear programming model, and (3) performing piece-wise linear delta approximations on the individual reliability functions of the components subject to repair. The piece wise linear delta approximation approach used employed surrogate piecewise affine functions defined over breakpoints to model the nonlinear reliability functions with a guaranteed margin of error [342]. It optimized: (1) the number of breakpoints, and (2) the location of the breakpoints. The nonlinear reliability functions were approximated within an absolute margin of 0.02 and they are displayed in Figure 21, Figure 22, Figure 23, and Figure 24.

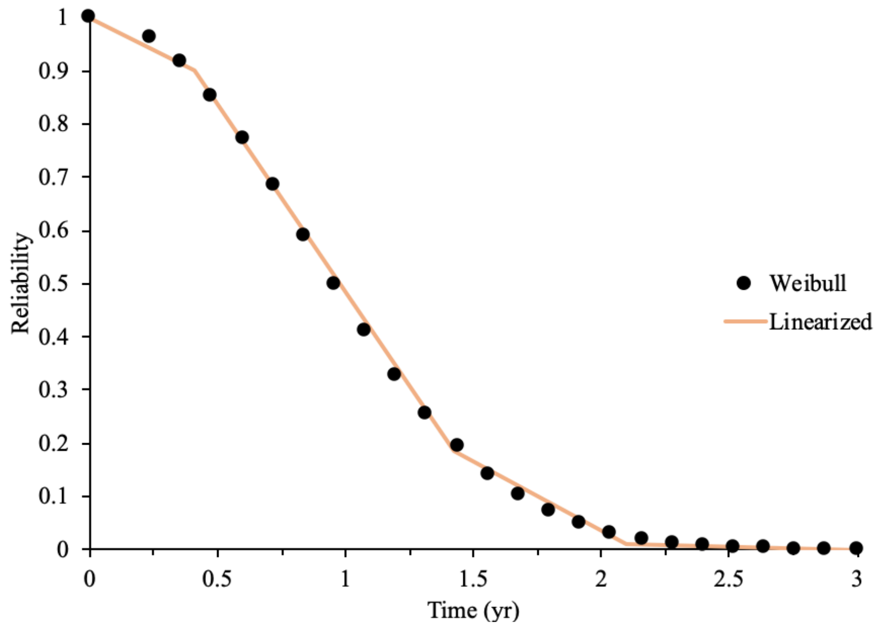


Figure 21: Centrifugal pump reliability curve

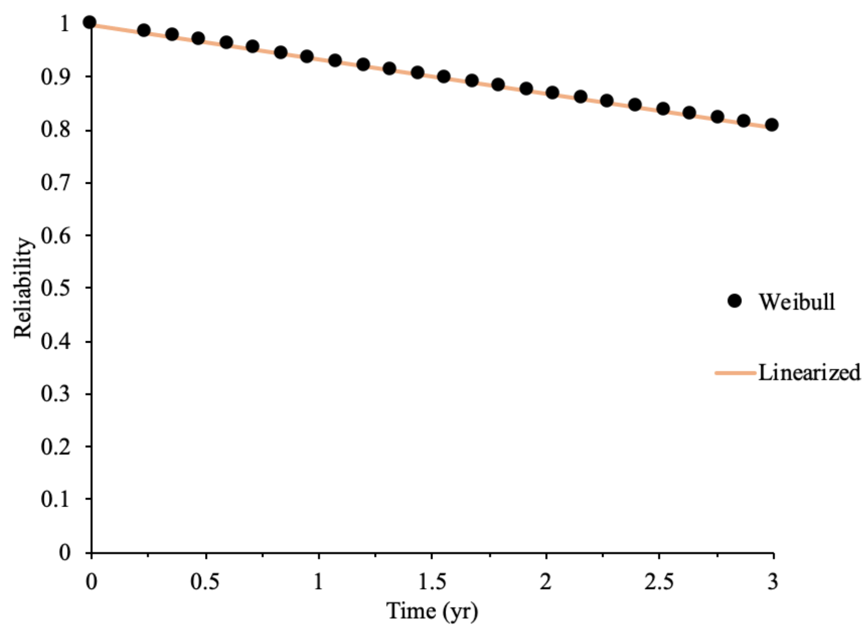


Figure 22: Isolation valve reliability curve

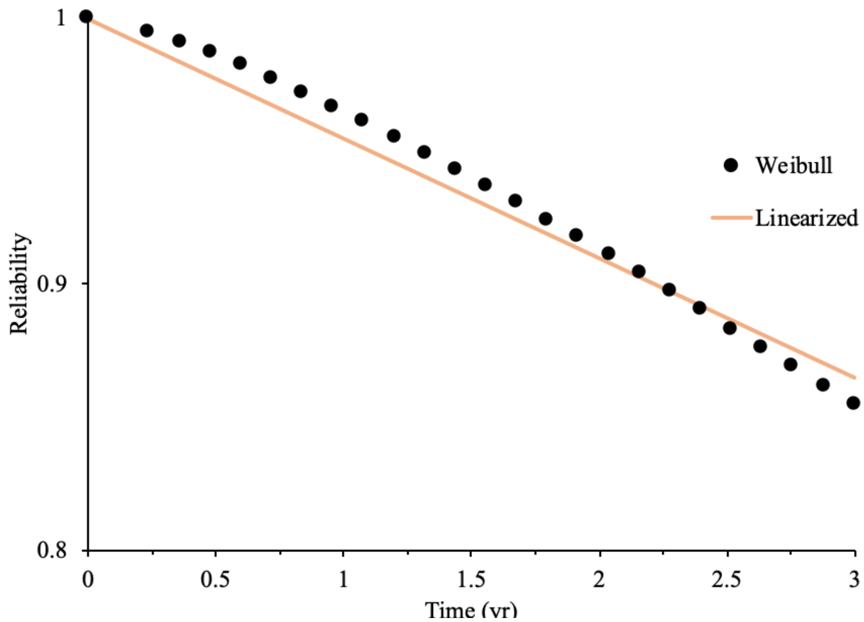


Figure 23: Automated control valve reliability curve

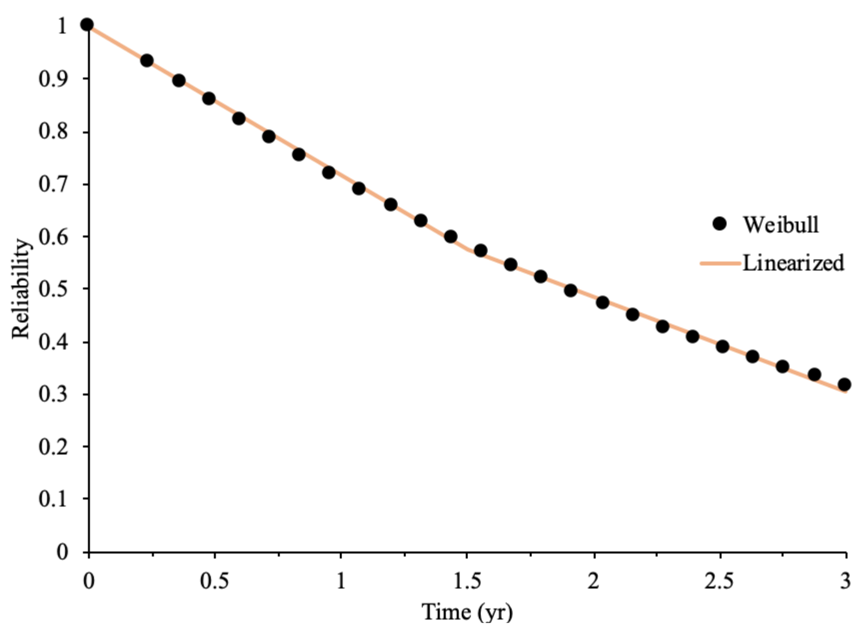


Figure 24: Manual control valve reliability curve

4.4.2.3. Maintenance Planning

The use of scenarios makes representation of the maintenance plan non-intuitive due to the maintenance actions being scenario-dependent binary variables in the second case study. However, insights can be seen from the resultant system reliability curves. A reliability curve for the intermediate reliability threshold of 0.8 is thus provided in Figure 25 to illustrate the results.

The system reliability is observed to decrease over time until it approaches the set reliability threshold. It is noted that the initial age of the components was set to zero however this adjustable. It can be seen that the scenarios with a higher degree of imperfect maintenance correspond to lower system reliability. It can be seen that the system reliability is maintained above the threshold in all three scenarios over the time horizon. Given that the optimal solution for this threshold showed that no replacement actions were required, this represents a useful insight for decision makers to avoid any unnecessary procurement expenditure. In the offshore environment which additionally suffers from limited storage space, limiting procurement without sacrificing reliability is highly desirable.

The model was run for different levels of system reliability as shown in Figure 26. It was observed that a significant increase in system reliability could be obtained via marginal increases in cost at lower levels of reliability. This method thus provides the decision maker with sensitivity analysis to assist them in visualizing the cost of different maintenance plans while accounting for variability in the quality of maintenance actions.

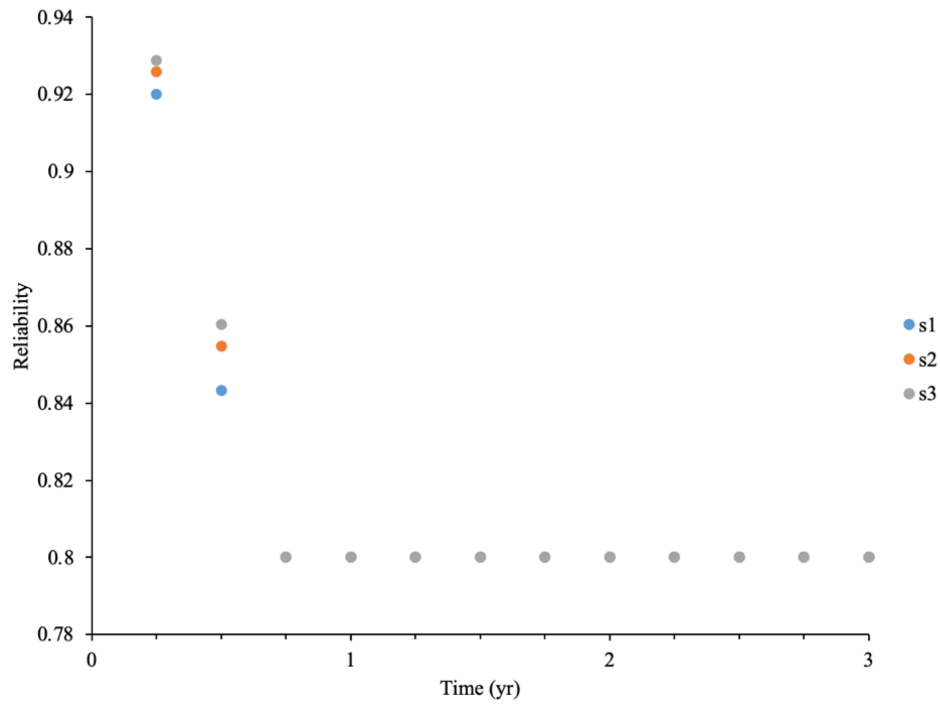


Figure 25: Case Study 2 – System reliability curve

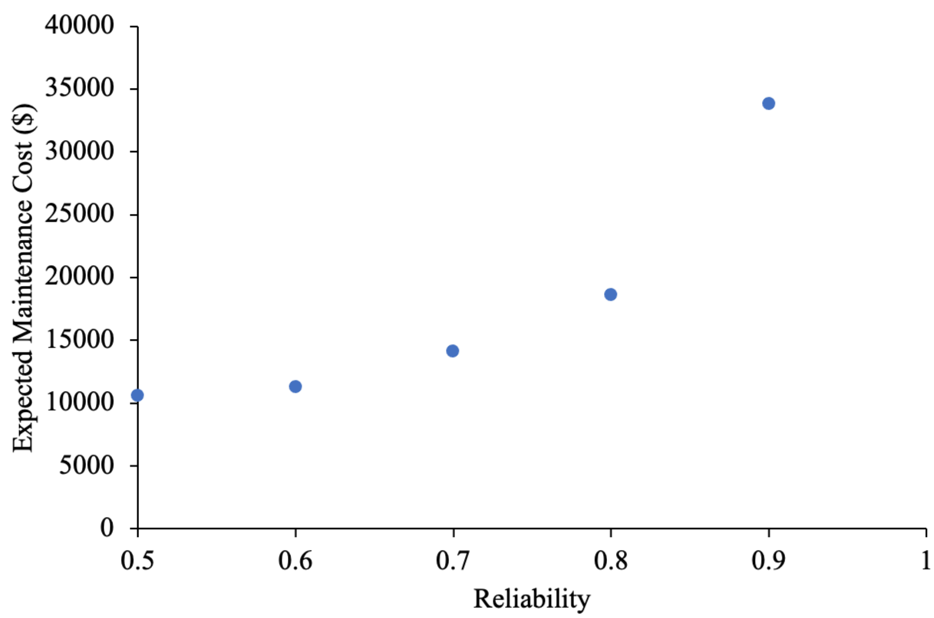


Figure 26: Case Study 2 - Optimal maintenance plans

4.5. Conclusion

Maintenance planning is complicated by resource scarcity, system complexity, reliability nonlinearity and parametric uncertainty. This paper presents a employs multi-objective optimization under uncertainty to help guide resource allocation. The approach was illustrated with a theoretical three-pump system and an offshore cooling water system.

The results showed that application of the techniques adopted in this paper can result in improvements in equipment and system reliability as compared to implementation of a manufacturer recommendation. The results also helped illustrate the tradeoffs between expected cost and system reliability.

The maintenance planning optimization approach used here can be adapted to ageing productive systems in different industries inclusive of refining, chemical production, and manufacturing both onshore as well as offshore.

It is noted that this approach can lead to significant complexity, combinatorial explosion, and computational intractability for series-parallel and other system configurations with a significant number of components. However, this methodology is amenable to the use of rolling horizon algorithms to help address such computational burdens. It is also further noted that data-driven failure prediction methods represent an alternative to tackling the uncertainty in reliability through their ability to develop custom equipment reliability models from non-generic condition and operational data using machine learning.

5. DATA-DRIVEN FAILURE PREDICTION FOR MAINTENANCE AND PRODUCTION SCHEDULING*

5.1. Summary

Maintenance can improve the availability of ageing production systems and prevent process safety incidents. However due to system complexity, resource allocation is non-trivial. This research developed and applied a framework to obtain optimal future-failure aware and safety-conscious production and maintenance schedules. Ensembles of nonlinear support vector machine classification models were leveraged to predict the time and probability of future equipment failure from equipment condition data. Multi-objective optimization of expected profit and a safety metric was then used to determine optimal process and maintenance schedules. The results of this research were that the ensemble models had an average accuracy and F1-score of 0.987, that the ensemble models were more accurate and sensitive than the individual classifiers by 3 percentage points, and that Pareto-optimal process and maintenance schedules were obtained providing alternative solutions to the decision maker. This research involved optimal resource allocation to help improve safety and system effectiveness.

* The text, tables as well as figures in chapter are reprinted with permission and modified from Gordon, C. A. K.; Burnak, B.; Onel, M.; Pistikopoulos, E. N. Data-Driven Prescriptive Maintenance: Failure Prediction using Ensemble Support Vector Classification for Optimal Process and Maintenance Scheduling. Industrial & Engineering Chemistry Research 2020, 58, 19607-19622. Copyright 2020 American Chemical Society.

5.2. Introduction

System resilience refers to the ability of system to responds to failures and prevent, mitigate, and respond to process safety incidents [343]. System effectiveness is the holistic performance of a system as a function of its availability, reliability, and quality characteristics [2]. Compromised system effectiveness and system resilience can be catastrophic with costly consequences such as injuries, fatalities, asset damage, and losses to reputation.

Maintenance is at the nexus of system effectiveness and system resilience and is one way to improve overall system performance. Equipment failure occurs as a result of degradation due to usage and environmental conditions. The aim of maintenance is to counteract degradation and improve the availability of productive systems. Examples of maintenance actions include cleaning, repair, and replacement.

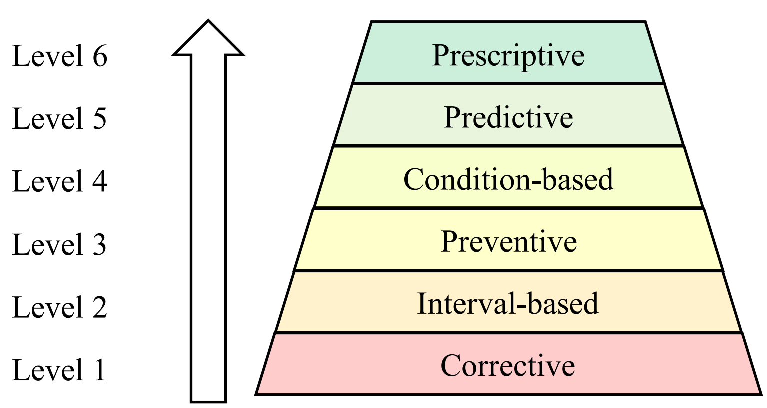


Figure 27: Types of maintenance. Reprinted with permission from [52].

The decisions of when and where to maintain are often non-trivial. At the component level, equipment failure behavior can be challenging to anticipate, and difficult to capture with high-fidelity first-principles models. At the system level, numerous nonlinear component interactions lead to complexity and decision multiplicity. These are exacerbated by resource limitations. As such, several approaches to maintenance have emerged and are shown in Figure 27.

Maintenance decision approaches can be categorized based on the data they leverage and their underlying mechanisms. Although some overlap occurs between them, they can be organized based on their degree of proactivity, complexity, and accuracy. Corrective maintenance is an approach in which actions are reactively done after equipment failure. The other approaches can be described as proactive with actions taken ahead of equipment failure. Interval-based maintenance involves actions taken on fixed intervals based on failure time data and engineering judgement. Preventive maintenance involves the use of nonlinear parametric models derived from equipment failure times to determine maintenance times. Condition-based maintenance involves statistical trend analysis of measurements of equipment health such as thickness, vibration signals, or temperature to forecast degradation and determine failure times based on a threshold.

Predictive maintenance uses machine learning and statistical models to determine future equipment degradation, and failure times based on multiple types of data, namely both time and condition data, as well as other types of data such as data on work orders, environmental conditions, and process measurements. In the manufacturing industry, unplanned downtime translates to an estimated $50 billion per year [344]. Predictive maintenance is projected to be able to improve equipment uptime by 10-20%, reduce overall maintenance costs by 5-10%, and reduce time spent planning maintenance by 20-50% [344]. Prescriptive maintenance builds upon predictive maintenance by using predictions to recommend operating and maintenance decisions to counteract future equipment degradation and failure.

Data-driven prescriptive maintenance scheduling and production optimization touches upon several fields of research including process systems engineering and process safety. A focused and indicative summary of related research in the fields of process and maintenance optimization, risk-based maintenance, and failure prediction is highlighted in Table 16.

A number of approaches have been developed to quantify the level of safety associated with production. These include safety indices [318, 323], dynamic fault trees [304], Bayesian methods [297, 316], and simulation [336]. It is noted that dynamic systems can exhibit both time-dependence and spatial-dependence and that the present approach solely considers time-dependence. Ahmed and coworkers [130] combined failure probability and consequence into an index to determine a set of maintenance schedules for a gas absorption system. Similarly, Hameed and coworkers [155] developed a safety index to optimize the maintenance schedule of a liquid natural gas sweetening unit using a genetic algorithm.

Table 16: Selected related previous work. Reprinted with permission from [52].

Reference	Description
Process and Maintenance Optimization	
[145]	Planning and scheduling of production and preventive maintenance under uncertainty
[187]	Batch plant design under uncertainty via Markov analysis
[2]	Optimal planning and design of production and maintenance for system effectiveness
[199]	Condition-based maintenance scheduling using a gamma process minimizing cost
[216]	Data-driven maintenance scheduling
[118]	Planning and scheduling of operations and condition-based maintenance using degradation modeling and robust optimization
[9]	Maintenance policy selection, process optimization, and resilience analysis
Risk-Based Maintenance	
[158]	Maintenance optimization involving reverse fault tree analysis
[130]	Goal programming to optimize maintenance cost, availability, and reliability
[300]	Dynamic maintenance planning using a Bayesian network
[155]	Risk-based maintenance scheduling using a genetic algorithm
[345]	Risk-based multi-objective maintenance optimization
Failure Prediction	
[152]	Failure prediction and maintenance scheduling using neural networks
[164]	Data-driven predictive maintenance scheduling using a genetic algorithm
[29]	Asset health prediction using random forest
[133]	Data-driven predictive maintenance scheduling using classifiers and a genetic algorithm
[33]	Time to failure prediction using principal component analysis and regression algorithms
[135]	Production and maintenance scheduling under uncertainty using a degradation signal model
[346]	Simultaneous fault detection and diagnosis via nonlinear support vector machines

This research presents a process-agnostic framework for optimal prescriptive maintenance. The framework involves equipment failure prediction using machine learning, consideration of process safety using a safety metric, and process and maintenance scheduling using mathematical optimization. The framework is applied on a motivating example and on a case study to simultaneously maximize system effectiveness and system resilience to determine optimal operations and maintenance decisions using multi-objective mixed-integer nonlinear programming. New features of the methodology include: the use of probabilistic ensemble voting for failure prediction, and the explicit incorporation of safety into prescriptive maintenance scheduling. Key features of the proposed methodology include: development of ensembles of support vector machine classification models, the use of a k-out-of-n alarm policy, and multi-objective optimization of maintenance and process conditions to obtain a Pareto-optimal set of solutions.

This section concludes with a problem statement. The remainder of this paper is organized as follows. Section 2 introduces the framework and details the methodology. Section 3 illustrates the work with an example and a case study. Section 4 then concludes the paper.

5.2.1. Problem Statement

The problem that the present research seeks to address is summarized below.

Generalized System

A process network involving species $i \in I$, equipment $j \in J$, process streams $s \in S$, utilities $u \in U$, time intervals $t \in T$, and system resilience thresholds $l \in L$.

Objectives

- Maximize system effectiveness
- Maximize system resilience

Given

- Process network design
- Equipment condition, maintenance, failure, and error data
- Equipment mean time to repair (MTTR)
- Production parameters
- Economic parameters
- Electricity, material, and human resource capacities

Determine

- Equipment failure time
- Production and maintenance schedules

Aspects of the problem are described through a simplified motivating example shown in Figure 28 and taken from [347]. The process network consists of a reactor in which a first-order exothermic reaction $A \rightarrow B$ occurs, a pump, and a water-cooled counter-flow heat exchanger.

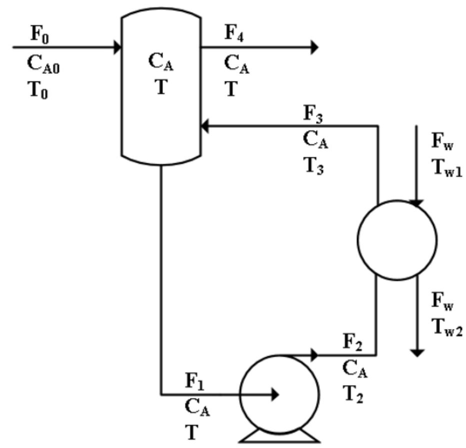


Figure 28: Motivating example. Reprinted with permission from [52].

It is desired to determine sets of flowrate, reactor temperature, and pump maintenance decisions that maximize expected profit subject to safety thresholds. It is noted that the interactions of production and maintenance decisions affect system effectiveness through their impact on conversion of A and expected profit, as well as affect system resilience through their impact on safety.

The approach used here seeks to perform future-failure aware and safety-conscious optimal prescriptive maintenance and process scheduling. Given pump data, the failure time of the pump can be predicted and used to prescribe an optimal sequence of flowrate, and temperature production decisions, as well as when pump repair is scheduled. This is done accounting for the safety consideration of maintaining the temperature of the reactor below given thresholds.

5.3. Methodology

5.3.1. Framework

The present approach is illustrated in the Prescriptive Optimization of Maintenance and Process Scheduling (PROMAPS) framework shown in Figure 29. Domain knowledge and data are fed in parallel to a safety model, and to a failure prediction model. The results from the safety model and failure prediction model are then used in a mathematical optimization model to obtain a set of optimized maintenance and process schedules. It is noted that the approach focuses on failure prediction and mathematical optimization. Each of the models is subsequently described in detail.

5.3.2. Safety

Process and maintenance decisions impact the level of safety associated with production. Safety metrics (SAM) can be introduced to help quantify the effect of process and maintenance decisions. A safety metric (λ_t) and aggregated safety metric (Λ) are used here in which the probability of failure (P_t^f) is obtained with the failure prediction, and the consequence of failure (C_t^f) is determined using a process-dependent consequence model [10]. The safety model consists of the functional form of the safety metrics, and is fed to the maintenance scheduling and process optimization model.

$$\lambda_t = P_t^f C_t^f \qquad \forall t \in T \tag{37}$$

$$\Lambda = \sum_{t \in T} \lambda_t \tag{38}$$

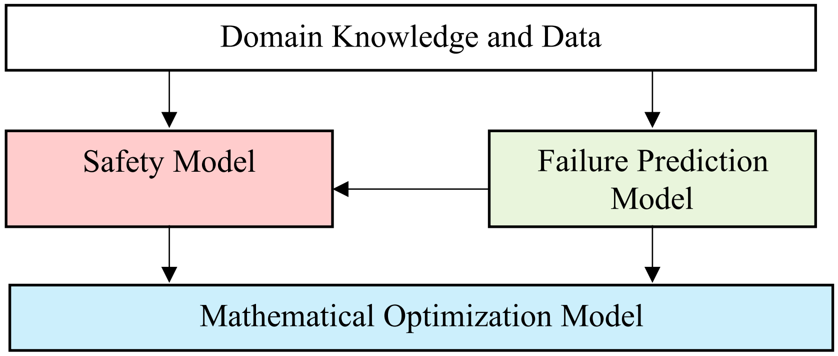


Figure 29: PROMAPS framework. Reprinted with permission from [52].

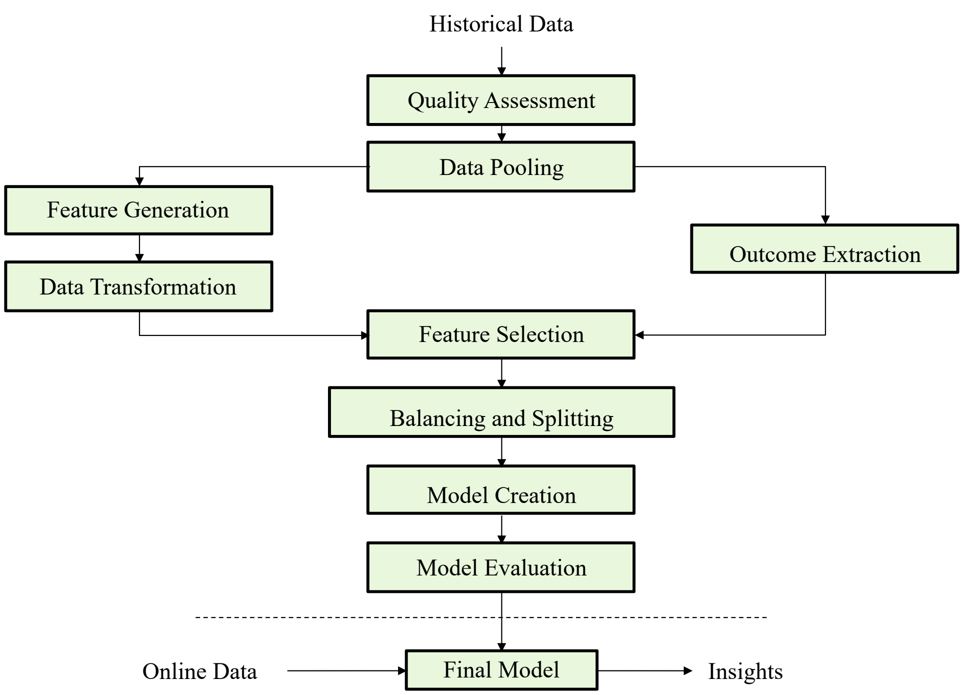


Figure 30: Overview of failure prediction methodology. Reprinted with permission from [52].

5.3.3. Failure Prediction

Support vector machine (SVM) classification is leveraged to predict future equipment failure. SVM classification has a number of advantages over other methods due to its ability to handle non-Gaussian distributed process data, categorize nonlinearly separable data through transformation to a higher-dimensional space, and to be represented as a convex optimization problem and solved to global optimality [346]. Readers interested in further details on support vector machines are directed to relevant resources [20, 23].

An overview of the failure prediction model development and use is shown in Figure 30. The approach consists of two phases: an offline development phase, and an online prediction phase.

The offline development phase begins with importing, assessing, and consolidating historical data. It is stressed that the input to the models are multiple types of data such as time, condition, process, and maintenance data. The data can consist of multiple data sets from different sources and time scales. The data sets used here were tabular and had a common feature of sample time. This was leveraged to pool the data into single data set with features sampled over shorter time scales repeated. In the event of missing data due to sensor error or underreporting, data can be cleaned by removing samples, or augmented via imputation.

The output of the data pooling step is a larger data set describing the historical trajectory of a piece of equipment. Each sample of the larger data set contains input features such as condition and maintenance features, and output features such as the time that the equipment would fail next.

The input feature data is subjected to feature generation and data transformation steps. Feature generation is used to create complementary additional features from the initial set of input features. The generated features are of two types: (1) features generated from domain knowledge such as the time since the last maintenance (TsLM) and leading indicators such as the number of errors since the last maintenance (EsLM); and (2) statistical features for each of the initial numeric input features to capture trends in the data such as mean, min, max, standard deviation, and root mean squared (RMS) computed over a sliding window. The generated feature data is then appended to the original initial input features to create an augmented input feature data set. The data is then transformed using Z-score normalization to facilitate analysis by including information about deviation from baseline operating conditions relative to average process variability.

The output feature data, namely the next time to failure data, is subjected to an outcome extraction step. This step involves the creation of a set of $\mathrm{N_k}$ features, each of which is a binary outcome vector ($\mathbf{Y_k}$) that indicates whether or not each sample would correspond to a failure within the next k hours where $\mathrm{k} \in \mathrm{K} = \{1,2, \ldots, \mathrm{N_k}\}$. For example, for $\mathrm{N_k} = 168$, this corresponds to determining whether or not there would be a failure in the week following the time of the sample.

The augmented input feature data is then combined with each of the N_k extracted binary outcome vectors to create N_k data sets. Each of these data sets is then fed through a feature selection step. The feature selection consists of statistical feature selection, through removal of any transformed generated features on the basis of variance, and wrapper feature selection via recursive feature elimination using a random forest classification algorithm. Random forest classification involves the construction of multiple decision trees, and was leveraged for feature selection due to its inherent ability to successively select the features on which to branch upon [20]. It is noted that the N_k classifiers can have different sets of selected features. The result of the feature selection step is N_k preprocessed data sets that each have one of the N_k outcome vectors and the corresponding selected augmented input features.

The final steps prior to model creation are balancing, and splitting. The preprocessed data sets are balanced by extracting all the samples that would correspond to failures, and then extracting an equal number of samples that would not correspond to failures based on random sampling from a uniform distribution. These balanced data sets are then split into training sets and validation sets using a 75:25 ratio. The training set is used for model creation, whereas the validation set is not used for model creation but instead for model evaluation.

Model creation was done on the basis of accuracy using nonlinear support vector machines with a radial basis function kernel and three repetitions of 10-fold cross validation. The models were tuned using grid search with accuracy as a model selection metric. A total of N_k models were created using each of the N_k training sets. For example, with $N_k = 168$, A total of 168 classifiers are created to predict failure within the each of the next $k = 1, 2, \dots, 168$ hours. These models were then evaluated to determine their performance on unseen data using the validation data sets with performance metrics of accuracy, sensitivity, specificity, and kappa.

The online prediction phase uses the created and evaluated models to predict the hour in which the equipment will next fail. N_s samples constituting a sampling horizon are aggregated and then fed to each of the N_k SVM classifiers. The classifiers output N_k binary numbers indicating whether or not failure is predicted to occur within each prediction horizon, as well as a corresponding N_k cumulative probabilities of failure based on Platt scaling [348].

To improve the robustness of predictions and reduce false positives, ensemble models are used. Each ensemble model consists of N_G successive individual models $\gamma \in \Gamma = \{1,2 \dots, N_G\}$, and the individual models used for the ensemble models are subsets of the N_k individual SVM classifiers. Ensemble models (G_q) are constructed for time periods $q = 1,2, \dots, (N_k - N_G + 1)$. Each ensemble is used to obtain an ensemble probability of failure (P_e^f) by combining the individual probabilities of failure (P_γ^f). The ensemble probability of no failure is the product of the individual probabilities of no failure within the ensemble, in an approach similar to considering the models in the ensemble as systems in parallel [18].

$$P_e^f = 1 - \prod_{\gamma} \left(1 - P_\gamma^f\right) \tag{39}$$

A failure alarm signal is generated if the ensemble probability of failure exceeds a threshold of 99.9999%. It is noted that this relatively strict threshold was selected to help avoid false positives and that other thresholds can be defined. Multiple failure alarm signals are combined using a k-out-of-n voting policy in which if k alarm signals are generated within a shifting horizon of n time periods, the first of the n time periods is outputted as the failure time prediction.

The outputs of the online prediction phase are a failure time prediction, and a cumulative probability of failure distribution. It is noted that the output is an implicit degradation trajectory, and corresponds to a remaining useful life distribution.

5.3.4. Mathematical Optimization

The mathematical optimization approach involves the development of a constrained multi-objective mixed-integer programming model. Objective functions (J_1 and J_2) represent a selected system effectiveness metric and a system resilience metric respectively. The model involves continuous decisions ($\mathbf{x}$) and binary decisions ($\mathbf{y}$) related to production and maintenance. These decision variables are related by equations ($\mathbf{g}$), maintenance constraints ($\mathbf{h}_1$), safety constraints ($\mathbf{h}_2$), and process constraints ($\mathbf{h}_3$). A generalized model is shown in (40).

It is stressed that the constraints in (40) are general and process-agnostic and that constraints relating to specific individual case studies, such as material balances and resource constraints, can be added to set of process constraints.

$$
\begin{aligned}
&\max \mathbf{J}(\mathbf{x},\mathbf{y}) = [\mathrm{J}_1(\mathbf{x},\mathbf{y}), \mathrm{J}_2(\mathbf{x},\mathbf{y})] \\
&\text{s.t.} \\
&\mathbf{g}(\mathbf{x},\mathbf{y}) = 0 \\
&\mathbf{h}_1(\mathbf{x},\mathbf{y}) \leq 0 \\
&\mathbf{h}_2(\mathbf{x},\mathbf{y}) \leq 0 \\
&\mathbf{h}_3(\mathbf{x},\mathbf{y}) \leq 0 \\
&\mathbf{x} \in \mathbf{X} \subseteq \Re^{\mathrm{n}} \\
&\mathbf{y} \in \mathbf{Y}\,\{0,1\}^{\mathrm{m}}
\end{aligned}
\tag{40}
$$

The outputs of the failure prediction methodology are a predicted future equipment failure time, and a probability of failure distribution. These outputs are fed to the mathematical optimization model as parameters to influence scheduled maintenance actions through the maintenance constraints. The output of the safety methodology are functions, and these are used to construct the safety constraints. This model is then solved using the epsilon-constraint method [26] to generate a set of safety thresholds, and process and maintenance schedules that contain optimized process and maintenance decisions. The major steps of the approach are summarized in Table 17.

Table 17: Summary of key aspects of the overall methodology. Reprinted with permission from [52].

#	Phase	Input	Steps	Output
1	Preprocessing	Historical data	Quality assessment, pooling, feature generation, Z-score normalization, outcome extraction	N_k data sets
2	Feature Selection	N_k data sets	Recursive feature elimination	N_k data sets, with fewer features
3	Balancing and Splitting	N_k data sets, with fewer features	Sampling, 75:25 data splitting	N_k training and validation data sets
4	Model Creation	N_k training sets	Nonlinear SVM, 10-fold cross-validation, tuning	Individual models
5	Prediction	N_G individual models, data	Ensemble creation via equation (39), use of probability threshold and k-out-of-n alarm policy	Probability of failure trajectory and failure time
6	Safety Quantification	Process description	Safety metric selection	Safety metric function
7	Scheduling	Failure prediction, safety metric function	Mathematical optimization, epsilon-constraint method	Future-failure aware safety-conscious process and maintenance schedules

5.4. Results

The first case study is the previously presented motivating example, and focuses on providing a summary of implementation of the main aspects of methodology on a hypothetical system. The interested reader is directed to the supporting information for additional details. The second case study is a more complex hydrocarbon separation system example, and focuses on illustrating the methodology in greater depth. The failure prediction models and data used for the hydrocarbon separation system pump are used for the hypothetical motivating example pump, and it is noted that there is an implicit assumption that the mechanical failure behavior of the pumps would be similar. In both case studies, the failure prediction was performed in R, and the mathematical optimization was done in GAMS 27.1.0 directly using the ANTIGONE solver [349]. This section proceeds by presenting the model creation results, followed by the two case studies.

5.4.1. Failure Prediction Model Creation

5.4.1.1. Feature Selection

The failure prediction methodology was applied to simulated historical data [350] to generate future equipment mechanical failure predictions. The data describes the mechanical failure of a generic piece of rotating equipment with similar mechanical failure behavior to that of a pump and is used for illustration purposes to demonstrate the approach. It consists of data on equipment error, failure and maintenance time, as well as condition data collected over a time horizon of one year. The condition data used consists of voltage, rotation, and vibration data and was sampled hourly. Twelve samples were selected from the data for each of the case studies to mimic online data for the prediction phase. Once consolidated and pre-processed, the data was split into two according to a 3:1 ratio. The first and larger set resulting from the split was the training set used to create the models. The second and smaller set from the split was the test set used to evaluate the models.

The data was used to build 168 classifiers. Feature generation led to a total of 30 features with features and transformations shown in Table 18. Feature selection via recursive feature elimination and random forest classification yielded a reduced set of features for each classifier with a median of 18 selected features across the 168 classifiers. A summary of the different features, and their prevalence across the classifiers is shown in Figure 31. The features selected most often were the rolling minimum of vibration, the features relating to the time since last maintenance, and the features relating to the number of errors since the last maintenance.

5.4.1.1. Model Evaluation

The failure prediction models were evaluated on validation data that was not used to train the models. The performance of the models across the prediction horizon can be seen in Figure 32 and Figure 33. It is noted that the performance of the first few individual models is worse than that of the others, and this could be due to them being trained with less sampled data. On the other hand, the performance of the ensemble models is observed to be more consistent than the individual models.

Table 18: Overview of features. Reprinted with permission from [52].

Original Features	**Transformations**
Voltage	Min
Rotation	Max
Vibration	Mean
Errors since last maintenance (ESLM)	Standard deviation (stdev)
Time since last maintenance (TSLM)	Root-mean squared (RMS)

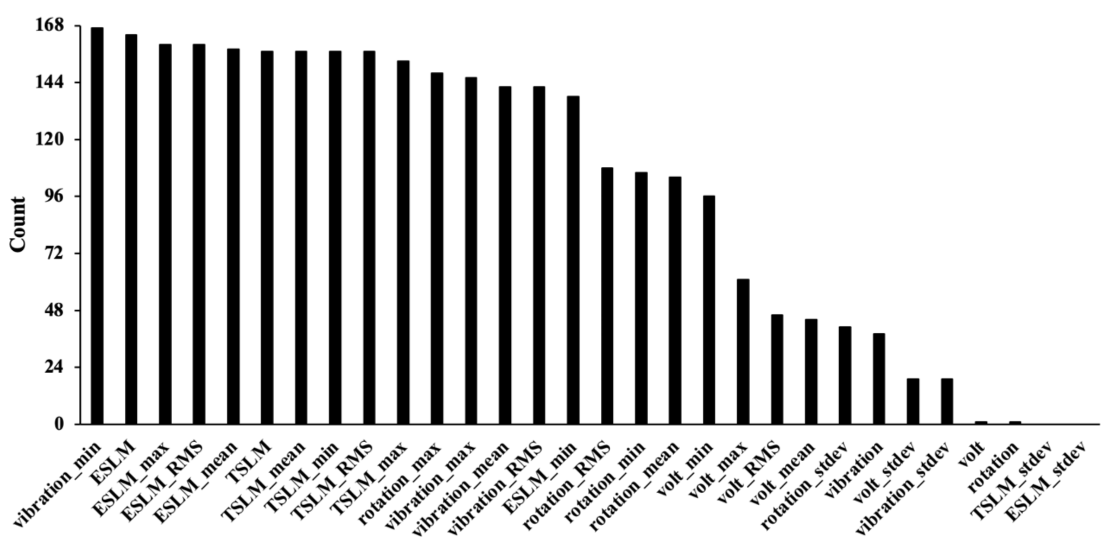


Figure 31: Aggregated feature selection results. Reprinted with permission from [52].

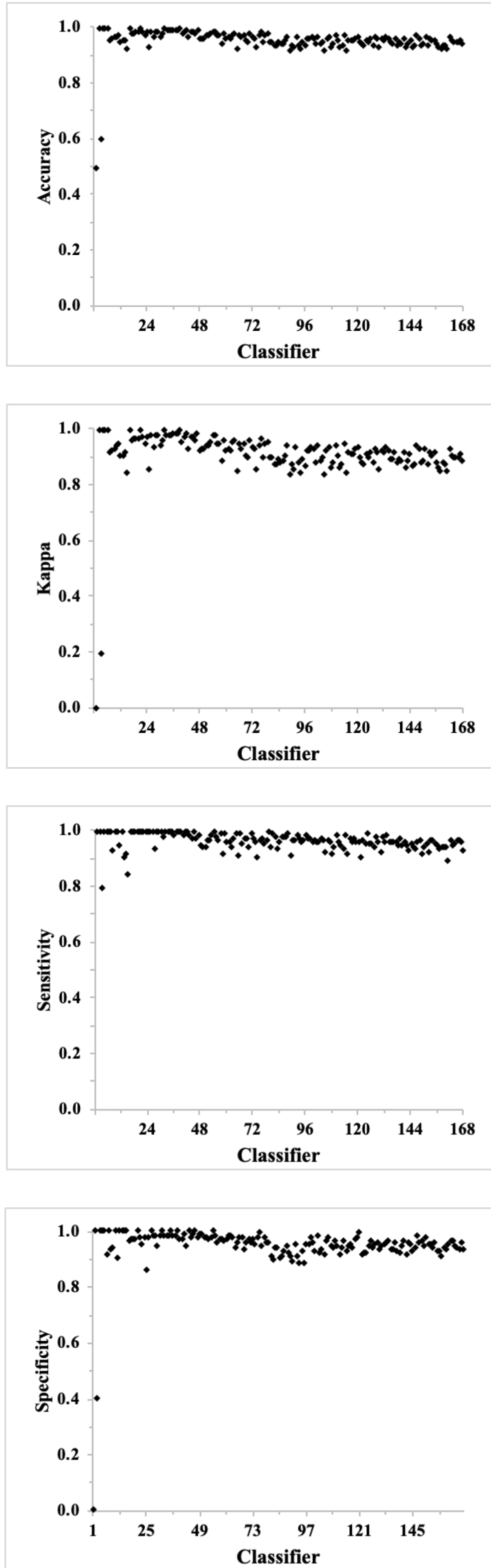


Figure 32: Performance of the individual models. Reprinted with permission from [52].

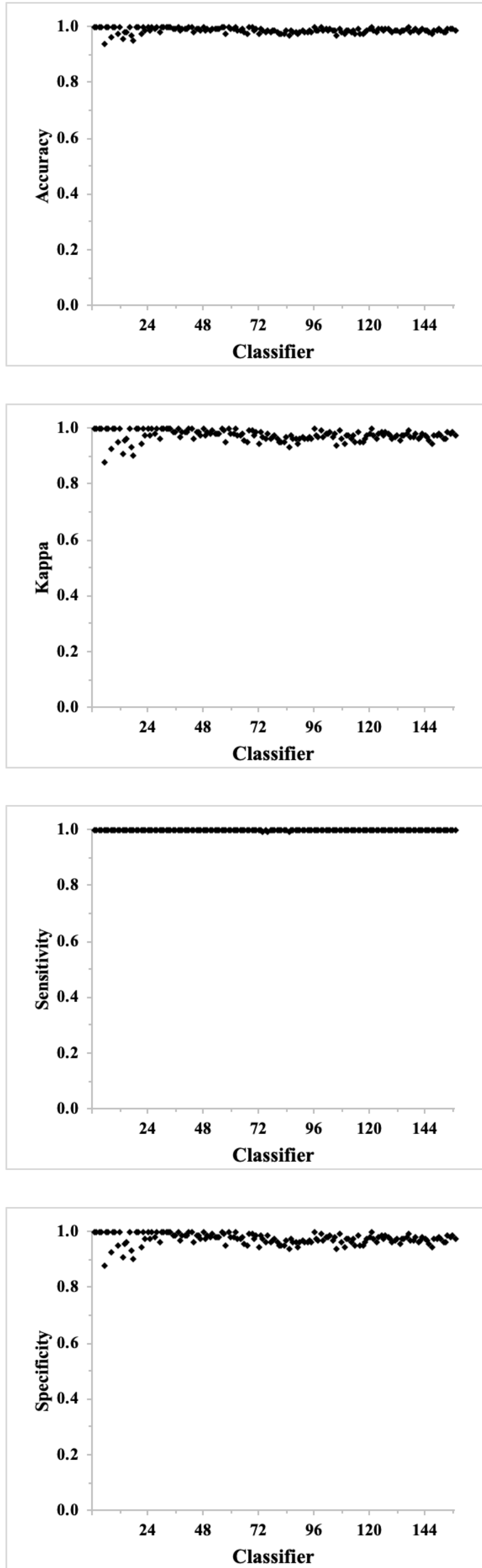


Figure 33: Performance of the ensemble models. Reprinted with permission from [52].

Table 19 reports the average model performance of the 168 individual models, as well as the average model performance of the 157 ensemble models created according to the described methodology. The results show that across all selected model evaluation metrics, the average performance of the ensemble models was higher than that of the average performance of the individual models. In particular, the use of the ensemble models increased accuracy by 3 percentage points, increased the sensitivity by 3.3 percentage points, and increased the specificity by 2.7 percentage points. The increases in these model performance metric values is significant, as they would correspond to cost-savings due to fewer false alarms and fewer missed threats. These results highlight the additional robustness imparted by the present methodology.

The ensembles of failure prediction models were then used to predict failure times in the case studies for use in production and maintenance scheduling.

Table 19: Aggregated model performance. Reprinted with permission from [52].

Metric	**Individual Models**	**Ensemble Models**
Accuracy	95.7%	98.7%
Kappa	91.4%	97.4%
Sensitivity	96.6%	100.0%
Specificity	94.7%	97.4%
F1	95.9%	98.7%
Precision	95.3	97.5%

5.4.2. Case Study 1

5.4.2.1. Description

The process system used for this case study was shown in Figure 28 and consist of a reactor, pump, and heat exchanger. The scheduling horizon is one week (168 hours), with an hourly time discretization. Parameters used for the case study can be found in the supporting information.

5.4.2.2. Failure Prediction

The developed failure prediction models were applied to online data to generate insights into failure. The predicted probability of failure trajectory is shown in Figure 34 for the individual models and in Figure 35 for the ensemble models. It can be observed that the ensemble model trajectory is smoother and the incidence of failure more evident. Application of a 9-out-of-10 alarm policy at a certainty threshold of 99.9999% yielded a failure time of 129 hours which has been shown on the figures.

5.4.2.3. Model Formulation

The problem statement for the optimization model is provided as follows. Given a predicted pump failure time and the system parameters defined in the supporting information, it is desired to determine a set of process and maintenance schedules that optimize expected profit and safety. It is assumed that feed flowrate is constant, repair restores equipment to an as-good-as-new condition, and that the outlet stream conditions are the same as the conditions within the reactor.

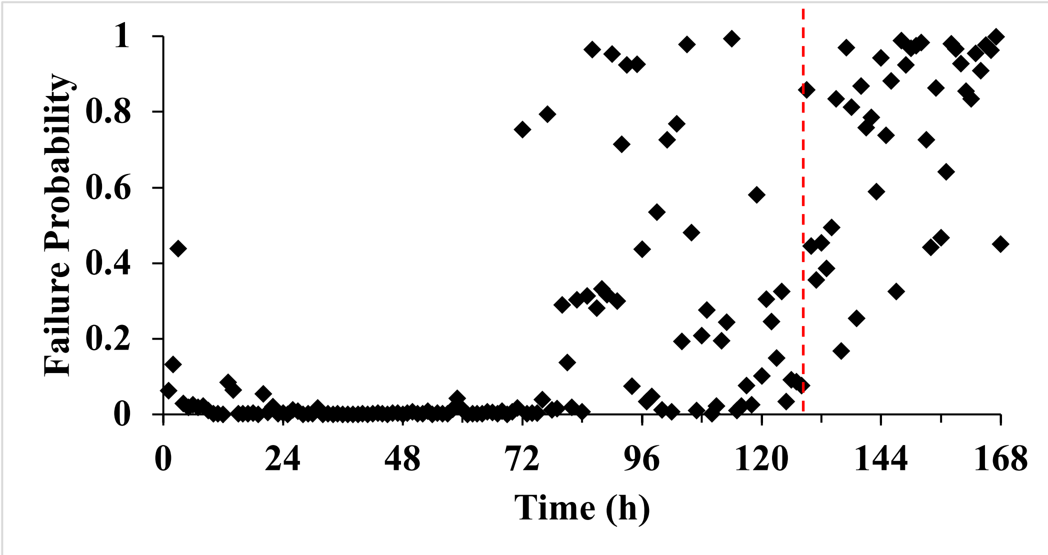


Figure 34: Case Study 1 – Individual model failure probabilities. Reprinted with permission from [52].

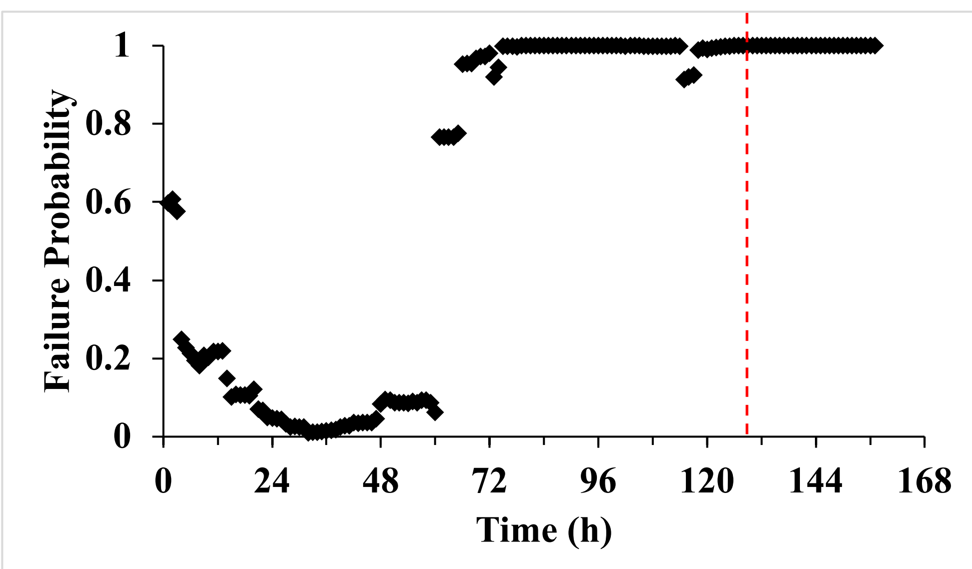


Figure 35: Case Study 1 – Ensemble model failure probabilities. Reprinted with permission from [52].

The model formulation involves species $i \in I = \{A, B\}$, process streams $s \in S = \{1,2,\dots,N_s\}$, equipment $j \in J = \{1,2,\dots,N_j\}$, time intervals $t \in T = \{1,2,\dots,N_T\}$, utilities $u \in U = \{1,2,\dots,N_u\}$, and system resilience thresholds $l \in L = \{1,2,\dots,N_l\}$. The expected profit ($\Phi$) is described as a function of the probability that the pump does not fail ($P_t^{s,sys}$), feed flowrate ($F_{0,t}$), conversion (χ_t), cooling water flowrate ($F_{w,t}$), and pumped recycle flowrate ($F_{2,t}$). The key continuous decision variable is reactor temperature ($\mathbb{T}_t$), and the key discrete decision variable is pump maintenance (m_t). Application of the epsilon-constraint method to maximize expected profit and safety leads to (42). The safety consideration here is for the temperature of the reactor to be below a temperature threshold ($\mathbb{T}_t^U$) by given margins ($\mathbb{T}_t^\Delta$). The rest of the formulation consists of (43) - (57) and involves sets of time intervals leading up to and including the current time interval (T_t^*), the number of intervals leading up to and including the current time interval ($\overline{\overline{T_t^*}}$), and sets of time intervals the length of the mean time to repair ($\overline{T}_t$).

Once implemented, the model consists of 2185 variables, comprising 1681 continuous variables and 504 binary variables, and 2690 constraints and is a mixed-integer nonlinear programming model.

$$\max \Phi = \sum_{t\in T} P_t^{s,sys}\left[100F_{0,t}\chi_t - 1.76F_{w,t} - 7.056F_{2,t}\right] \tag{41}$$

$$\mathbb{T}_t^U - \mathbb{T}_t \geq \mathbb{T}_t^\Delta \tag{42}$$

$$\chi_t = 1 - C_{A,t}/C_{A0} \qquad \forall t \in T \tag{43}$$

$$F_{0,t}\chi_t = Vke^{\left(\frac{-E}{R\mathbb{T}_t}\right)}C_{A,t} \qquad \forall t \in T \tag{44}$$

$$-\Delta H_t^{rxn}F_{0,t}\chi_t = F_{0,t}C_p\left(\mathbb{T}_t - \mathbb{T}_{0,t}\right) + Q_t^{HE} \qquad \forall t \in T \tag{45}$$

$$F_{2,t}C_p\left(\mathbb{T}_{2,t} - \mathbb{T}_{3,t}\right) = F_{w,t}C_p^w\left(\mathbb{T}_{w2,t} - \mathbb{T}_{w1}\right) \qquad \forall t \in T \tag{46}$$

$$Q_t^{HE} = AU\left[\frac{\left(\mathbb{T}_{2,t} - \mathbb{T}_{w2,t}\right) - \left(\mathbb{T}_{3,t} - \mathbb{T}_{w1}\right)}{\log\left[\left(\mathbb{T}_{2,t} - \mathbb{T}_{w2,t}\right)/\left(\mathbb{T}_{3,t} - \mathbb{T}_{w1}\right)\right]}\right] \qquad \forall t \in T \tag{47}$$

$$\mathbb{T}_{2,t} = \mathbb{T}_t \qquad \forall t \in T \tag{48}$$

$$\mathbb{T}_{2,t} - \mathbb{T}_{w2,t} \geq 11.1 \qquad \forall t \in T \tag{49}$$

$$\mathbb{T}_{3,t} - \mathbb{T}_{w1} \geq 11.1 \qquad \forall t \in T \tag{50}$$

$$F^L(1 - m_t) \leq F_{2,t} \leq F^U(1 - m_t) \qquad \forall t \in T \tag{51}$$

$$F_w^L(1 - m_t) \leq F_{w,t} \leq F_w^U(1 - m_t) \qquad \forall t \in T \tag{52}$$

$$\sum_{t\in \acute{T}} m_t^{start} = 1 \tag{53}$$

$$m_t^{prior} \geq \sum_{\tau\in T_t^*} m_\tau^{start} \qquad \forall t \in T \tag{54}$$

$$\sum_{\tau\in T_t^*} 1 - m_\tau^{prior} \geq \left(\overline{\overline{T_t^*}} - 1\right)m_t^{start} \qquad \forall t \in T \tag{55}$$

$$\sum_{\tau\in \overline{T}_t} m_\tau \geq m_t^{start}MTTR \qquad \forall t \in T \tag{56}$$

$$\sum_{t\in T} m_t \leq MTTR \tag{57}$$

5.4.2.4. Maintenance Scheduling and Process Optimization

The optimization model was implemented to obtain optimal values for the process and maintenance variables over the time horizon. It is noted that for this simplified system, the process schedules are effectively piecewise constant, and as such the results are summarized in Table 20. It can first be observed that increasing the safety margin generally decreased the conversion, reactor temperature, and expected profit. With the upper bound on temperature set at 389 K, it can further be observed that the solutions were non-dominated which corresponds to the epsilon constraints being active. In all the solutions, maintenance was scheduled sufficiently ahead of the predicted failure time.

This example explored multiple aspects of process variables, maintenance, and safety and it is expected that increased benefits of a prescriptive maintenance approach would be realized for larger systems with interacting failure-prone equipment. The paper proceeds with application of the methodology to a larger and more complex system.

Table 20: Case Study 1 – Results. Reprinted with permission from [52].

Margin (K)	Conversion	Reactor Temperature (K)	Maintenance Start Time (hr)	Expected Profit ($/week)
20	0.797	369	1	5.295e5
30	0.789	359	1	5.241e5
35	0.786	354	6	5.190e5
40	0.782	349	24	5.146e5
50	0.774	339	15	5.098e5

5.4.3. Case Study 2

5.4.3.1. Description

The process system used for this case study is a hydrocarbon separation system. An overview of the system is shown in Figure 36.

The feed stream (S1) to the overall system is a mixture of hydrocarbon species (A, B, C, and D) along with impurities (E). The hydrocarbon mixture is fed to a tower (T1) to be separated into distillate (S3), and a bottoms outlet stream (S2) rich in species C and D which undergo further downstream processing after passing through a reboiler (E2). The distillate is fed to a shell and tube heat exchanger (E1) where it is cooled, and used to preheat a process fluid. It then goes to a flash drum (V1) where it is separated into a gaseous phase and a liquid phase. The gaseous phase is vented through two rotary gas turbines (B1 & B2) to recover energy and then to a vessel (V2) for intermediate storage, removal of impurities to a waste management system, as well as controlled recycle of hydrocarbon fluid to the flash drum. The liquid phase is fed to two pumps (P1 & P2) and then split into a reflux stream, and into an outlet stream (S17) enriched in species B.

Pump integrity is critical to the overall safety of the hydrocarbon system. The two pumps are in parallel and alternately operated: when the primary pump (P1) is taken offline for testing or maintenance, the secondary pump (P2) is brought online. The failure mode considered is seal failure induced by mechanical failure of the primary pump. Mechanical failure can result in misdirection of force and resultant damage to pump seals. The scenario considered is the loss of containment of process fluid leading to a vapor cloud explosion.

The scheduling horizon is one week (168 hours), with an hourly time discretization. A summary of the parameters used for the case study can be found in the supporting information and include process parameters from Schenk and coworkers [351].

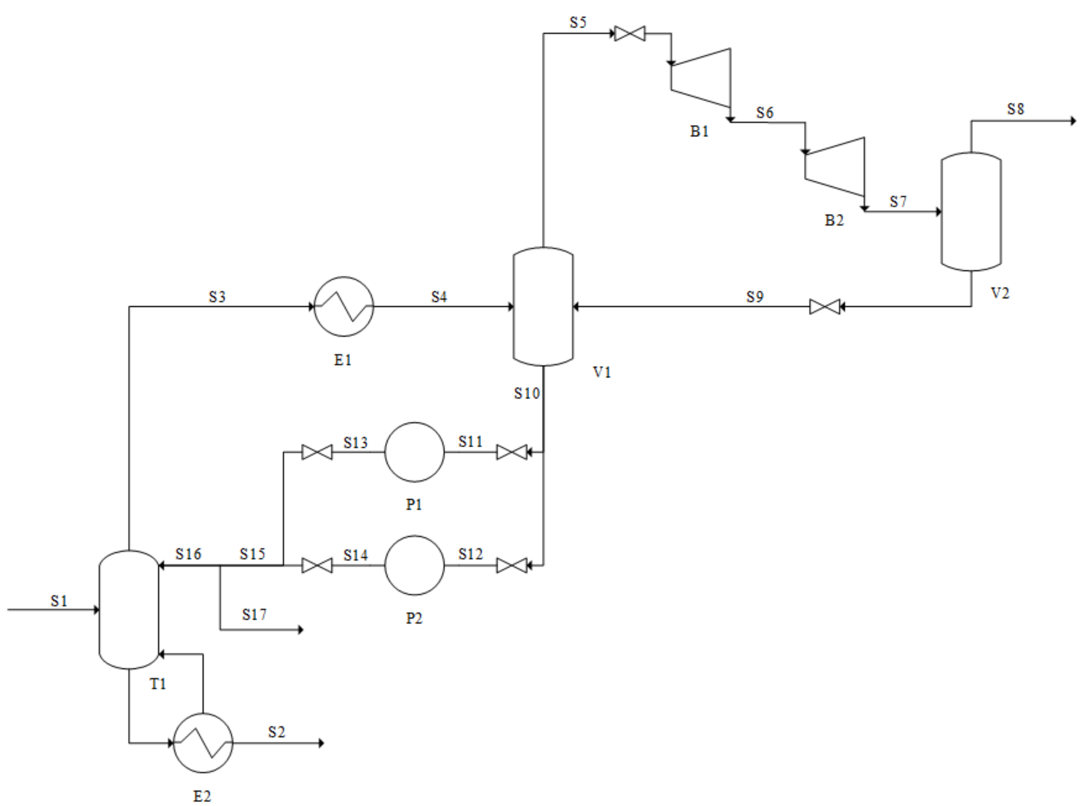


Figure 36. Hydrocarbon separation system. Reprinted with permission from [52].

5.4.3.2. Failure Prediction

The developed failure prediction models were applied to online data to generate insights into failure. The resultant failure probability trajectories are shown in Figure 37 for the individual classifiers and in Figure 38 for the ensemble models. A failure time prediction of 61 hours was determined using the described ensemble model methodology and the k-out-of-n alarm policy. It was seen that the predicted failure probabilities were generally low before the failure time, but then increased. It was also observed that the failure probability predictions were uniformly high after the predicted failure time. The likely incidence of failure at the predicted time due to accumulated degradation was then fed into the maintenance scheduling and process model for proactive and optimized action to prevent the equipment failure.

5.4.3.3. Model Formulation

The problem statement for the production and maintenance scheduling model is provided as follows. The objectives are to maximize system effectiveness and system resilience. It is assumed that: mean time to repair is deterministic, maintenance does not induce failures, and that the secondary pump experiences failure at a baseline rate. Information taken as being given are: the predicted failure time of the primary pump; the process network design; pump mean time to repair; production parameters; cost and revenue parameters; and electricity, material, and human resource capacities. The key continuous decision variables are the flowrates, and the key discrete decision variables considered are maintenance and availability of the primary pump.

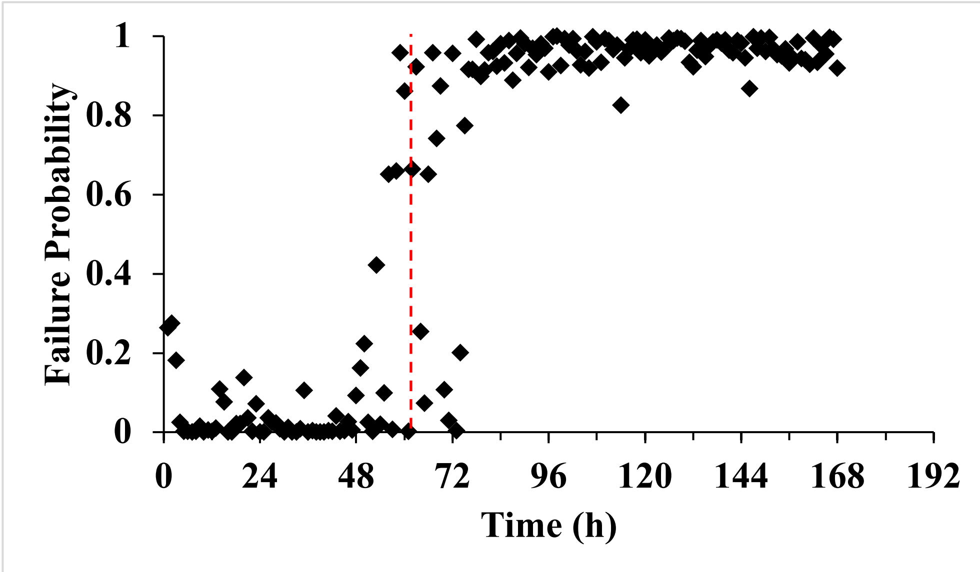


Figure 37: Case Study 2 – Individual model failure probabilities. Reprinted with permission from [52].

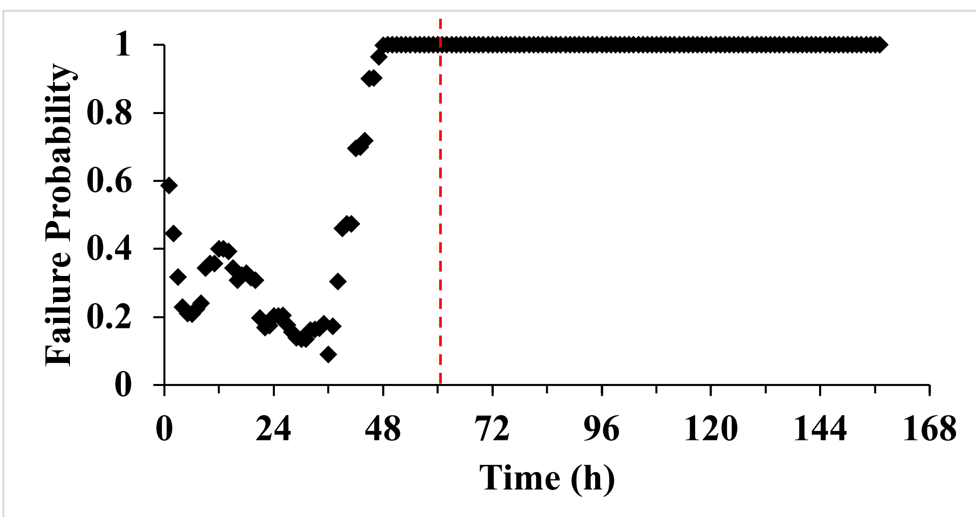


Figure 38: Case Study 2 – Ensemble model failure probabilities. Reprinted with permission from [52].

The model formulation involves species $i \in I = \{A, B, C, D, E\}$, process streams $s \in S = \{1,2, \ldots, N_s\}$, equipment $j \in J = \{1,2, \ldots, N_j\}$, time intervals $t \in T = \{1,2, \ldots, N_T\}$, utilities $u \in U = \{1,2, \ldots, N_u\}$, and system resilience thresholds $l \in L = \{1,2, \ldots, N_l\}$. The set of pumps is a subset of the set of equipment and is denoted $j \in J^P$. Once implemented, the model contains 6627 variables, comprising 4189 continuous variables and 2438 binary variables, and 10249 constraints. It is noted that McCormick relaxations are used for bilinear terms resulting in additional constraints and a mixed-integer linear programming model.

Objective

The multi-objective problem is transformed into single-objective problems maximizing system effectiveness subject to different system resilience constraints. The system effectiveness criterion considered here is expected profit.

$$\max \Phi = \sum_{t \in T} P_t^{s,sys} \left[\sum_{i \in I} V_i F_{i,t}^{out} - C^l HRU_t - C^m MRU_t - C^e ERU_t^{total} + \sum_{t \in T} C^e ERG_t - \sum_{u \in U} C^u Q_{u,t} \right] \tag{58}$$

The expected profit objective function contains six terms. The first term is the equivalent value of the species leaving the system, and consists of their marginal value (V_j) and flowrate of streams exiting the system ($F_{j,t}^{out}$). The second term is human resource cost, and consists of unit human resource cost (C^l), and human resources used (HRU_t). The third term is maintenance cost, and consists of unit maintenance cost (C^m), and maintenance resources used (MRU_t). The fourth term is electricity cost, and consists of unit electricity cost (C^e) and electricity resource used (ERU_t). The fifth term captures the power gained from the energy recovery turbines, and consists of unit electricity cost (C^e) and electricity resource gained (ERG_t). The sixth term is utility cost and consists of the unit utility cost (C^u), and the energy exchanged by the utility stream ($Q_{u,t}$). The probability of the system being in a non-failure state is denoted ($P_t^{s,sys}$) and is obtained using the predicted probability of failure of the pumps which are key system components. It is noted that maximizing the expected profit of the system corresponds to determining the set of decisions that maximize production revenue and minimize costs.

Safety constraints are obtained using the epsilon-constraint method. The obtained thresholds are reported in the supporting information and the constraints are shown in constraint (59). It is noted that use of the different thresholds corresponds to the addition of different safety constraints to the optimization problem. It is further noted that there are N_l single-objective problems, each of which correspond to determining the optimal maintenance and production schedules that maximize expected profit such that the aggregated safety metric (Λ) is less than a given threshold ($\overline{\Lambda}_l$).

$$\Lambda \leq \overline{\Lambda}_l \qquad \forall l \in L \quad (59)$$

The formulation is further constrained by process constraints, safety constraints, maintenance constraints, resource constraints, and variable bounds.

Process constraints

The equality and inequality constraints relating to production are defined for the overall process, and for each unit in turn. It is recalled that the process involves equipment $j \in J$ and process streams $s \in S$. Furthermore, a set of all equipment except for the tower ($\tilde{J}$), the sets of inlet streams to individual equipment (S_j^{in}) and outlet streams from individual equipment (S_j^{out}) are defined. The molar flowrates (F) of species entering and leaving equipment are described by (60).

$$\sum_{s \in S_j^{in}} F_{i,s,t}^{in} = \sum_{s \in S_j^{out}} F_{i,s,t}^{out} \qquad \forall i \in I, \forall j \in \tilde{J}, t \in T \quad (60)$$

The outlet flowrate of B is constrained to be between lower production targets ($PROD\_TARGET_t^L$) and upper production targets ($PROD\_TARGET_t^U$) by (61).

$$PROD\_TARGET_t^L \leq F_{B,t}^{out} \leq PROD\_TARGET_t^U \qquad \forall t \in T \quad (61)$$

The species molar feed flowrate ($F_{s1,i,t}$) is defined by a fixed molar feed composition ($FEED\_X_I$), and a variable feed flowrate ($F_{s1,t}$) constrained within design bounds ($FEED^L, FEED^U$) of ±10% of the nominal flowrates.

$$F_{s1,i,t} = (FEED\_X_I)F_{s1,t} \qquad \forall i \in I, \forall t \in T \quad (62)$$

$$F_{s1,t} = \sum_{i \in I} F_{s1,i,t} \qquad \forall t \in T \quad (63)$$

$$FEED^L \leq F_{s1,t} \leq FEED^U \qquad \forall t \in T \quad (64)$$

Surrogate modeling was used to describe the tower. This was done by constructing a high-fidelity model with nonlinear material, equilibrium, summation, and heat (MESH) equations in Aspen Plus, and then then performing Global Sensitivity Analysis (GSA) to obtain surrogate models for outcome variables as a function of input covariates within ±10% of their nominal values. The outcome variables were distillate species molar flow rates ($F_{s3,A}, F_{s3,A}, F_{s3,A}$) and temperature ($T_{s3}$). The input covariates were feed species molar flowrate ($F_{s1,A}, F_{s1,B}, F_{s1,C}, F_{s1,D}, F_{s1,E}$), feed temperature ($T_{s1}$), bottoms flowrate ($F_{s2}$), and reflux ratio (R).

The data for developing the surrogate models was obtained via Latin Hypercube Sampling (LHS) implemented in R using the lhs package. A sample hyperspace was defined using ±10% of the nominal values of the input parameters. A metaheuristic genetic algorithm with five generations and mutation probability of 0.125 was then used to maximize a harmonic-mean distance based S-optimality criterion, and obtain 100 sets of input covariate values to use in simulating 100 corresponding sets of outcome variables.

The surrogate models were then constructed using multivariate linear regression. Model training was done with 90% data, and 10% of the data was reserved for testing. The covariates for each of the surrogate models were selected based on their p-values at a significance threshold of 0.001, and based on their absolute magnitude at a size threshold of 0.001. The average mean-normalized root mean squared error for all the surrogate models was 2.8%. It is noted that the developed multivariate linear regression models are only valid within ±10% of the nominal values of the input parameters. The surrogate models were added as equality constraints.

$$F_{s1,A,t} = \beta_1 F_{s1,A,t} + \beta_2 R_t + \beta_3 \qquad \forall t \in T \quad (65)$$

$$F_{s3,B,t} = \beta_4 F_{s1,B,t} + \beta_5 F_{s1,C,t} + \beta_6 F_{s1,D,t} + \beta_7 R_t - \beta_8 F_{s2,t} + \beta_9 \qquad \forall t \in T \quad (66)$$

$$F_{s3,E,t} = \beta_{10} F_{s1,E,t} + \beta_{11} R_t + \beta_{12} \qquad \forall t \in T \quad (67)$$

$$T_{s3,t} = \beta_{13} F_{s1,C,t} - \beta_{14} F_{s2,t} + \beta_{15} \qquad \forall t \in T \quad (68)$$

An overall material balance for the tower is shown in (69). A slack variable (δ_t) was added to help model convergence and was observed to be on the order of 1%

in magnitude relative to the other total molar flows. Furthermore, equipment availability (a $\in \{0,1\}$) is introduced to constrain flow through the pumps.

$$F_{s1,t} + F_{s16,t} = F_{s2,t} + F_{s3,t} + \delta_t \qquad \forall t \in T \quad (69)$$

$$a_{P1,t}F^L \leq F_{s13,t} \leq a_{P1,t}F^U \qquad \forall t \in T \quad (70)$$

$$a_{P2,t}F^L \leq F_{s14,t} \leq a_{P2,t}F^U \qquad \forall t \in T \quad (71)$$

Safety constraints

The safety metric used for vapor cloud explosion is quantified through the TNT-equivalency method and the determined probability of failure [10, 14]. The safety metric (λ_t) is a function of flowrate ($F_{s15,t}$), release time (t^r), generic probability of seal failure ($P^{s,f}$), the predicted probability of mechanical failure ($P^{m,f}$), and other parameters reported in the supporting information. It is noted that a linear approximation to (74) is implemented within the range of flowrates corresponding to the design bounds. The dynamic safety metric is computed as a function of probability and consequence in (75) for each pump. The consequence of failure (C_t^f) selected here is scaled overpressure and corresponds to explosion damage and costs. The primary pump failure probability is calculated in (76), and the secondary pump failure probability is assumed to be baseline. It is noted that (76) corresponds to repair that is almost as-good-as-new. Furthermore, the column vapor flowrate exiting the first tray is constrained by (77) to avoid flooding.

$$m_t^{TNT} = \frac{1000\eta_{ex}\, F_{s15,t} t^r C_{p_B}}{E^{TNT}} \qquad \forall t \in T \quad (72)$$

$$z_t^{TNT} = \frac{r^{TNT}}{[m_t^{TNT}]^{1/3}} \qquad \forall t \in T \quad (73)$$

$$C_t^f = \frac{1616\left[1+\left(\frac{z_{TNT,t}}{4.5}\right)\right]^2}{\sqrt{1+\left(\frac{z_{TNT,t}}{0.048}\right)^2}\sqrt{1+\left(\frac{z_{TNT,t}}{0.32}\right)^2}\sqrt{1+\left(\frac{z_{TNT,t}}{1.35}\right)^2}} \qquad \forall t \in T \quad (74)$$

$$\lambda_t = P^{s,f} \cdot P_{P1}^f C_t^f + P^{s,f} \cdot P^{baseline} C_t^f \qquad \forall t \in T \quad (75)$$

$$P_{P1}^f = P^{m,f}\left(1 - m_{P1,t}^{prior}\right) + P^{baseline} m_{P1,t}^{prior} \qquad \forall t \in T \quad (76)$$

$$F_{s3,t} \leq F^{U,flood} \qquad \forall t \in T \quad (77)$$

Maintenance constraints

A number of constraints define whether or not to do maintenance on the pumps within a time interval ($m_{j,t} \in \{0,1\}$). Constraint (78) enforces that at most one pump is maintained at a time to avoid interrupting production. Maintenance is started at most once during the time horizon for each pump as shown in (79). Constraint (80) enforces that maintenance is started before the predicted failure time. Constraints (81) and (82) indicate whether maintenance has previously been performed within the time horizon. Once maintenance is started, it is constrained to last for the mean time to repair (MTTR) by inequalities (83) and (84). A pump is unavailable if it is under maintenance as seen in (85). Constraints (86) - (90) restrict the number of pump changeovers ($s_{j,t}$). Additional subsets of time intervals are introduced: the set of time intervals leading up to immediately before the predicted failure time ($\acute{T}$), the set of all time intervals except the last time interval ($\widetilde{T}$), sets of time intervals the length of the mean time to repair ($\overline{T}_t$), sets of time intervals leading up to and including the current time interval (T_t^*) where $\overline{\overline{T_t^*}}$ is the number of intervals leading up to and including the current time interval, the sets of the 8 time intervals after each time interval ($\breve{T}_t$), and the set of all but the last κ time intervals ($\widehat{T}$).

$$m_{P1,t} + m_{P2,t} \leq 1 \qquad \forall t \in T \quad (78)$$

$$\sum_{t \in T} m_{j,t}^{start} \leq 1 \qquad \forall j \in J^P, \forall t \in T \quad (79)$$

$$\sum_{t \in \acute{T}} m_{P1,t}^{start} = 1 \qquad (80)$$

$$m_{P1,t}^{prior} \geq \sum_{\tau \in T_t^*} m_{P1,\tau}^{start} \qquad \forall t \in T \quad (81)$$

$$\sum_{\tau \in T_t^*} 1 - m_{P1,\tau}^{prior} \geq \left(\overline{\overline{T_t^*}} - 1\right) m_{P1,t}^{start} \qquad \forall t \in T \quad (82)$$

$$\sum_{\tau \in \overline{T}_t} m_{P1,\tau} \geq m_{P1,t}^{start} MTTR \qquad \forall t \in T \quad (83)$$

$$\sum_{t \in T} m_{P1,t} \leq MTTR \qquad (84)$$

$$1 - a_{j,t} \geq m_{j,t} \qquad \forall j \in J^P, \forall t \in T \quad (85)$$

$$s_{j,t} \leq a_{j,t} + a_{j,t+1} \qquad \forall j \in J^P, \forall t \in \widetilde{T} \quad (86)$$

$$s_{j,t} \geq a_{j,t+1} - a_{j,t} \qquad \forall j \in J^P, \forall t \in \widetilde{T} \quad (87)$$

$$s_{j,t} \geq a_{j,t} - a_{j,t+1} \qquad \forall j \in J^P, \forall t \in \widetilde{T} \quad (88)$$

$$s_{j,t} \leq 2 - a_{j,t} - a_{j,t+1} \qquad \forall j \in J^P, \forall t \in \widetilde{T} \quad (89)$$

$$\sum_{\tau \in \check{T}_t} s_{j,t} \leq 1 \qquad \forall j \in J^P, \forall t \in \hat{T} \quad (90)$$

The constraints on maintaining the pumps are complemented by a set of constraints on equipment inspections ($u_{j,t}$) during the scheduling horizon. At most one inspection on each equipment during the horizon is enforced by (91), with each equipment to be inspected once (92). For safety, (93) enforces that no inspections be performed at the same time as pump repair. At most one equipment is to be inspected per shift where the sets of 12 time intervals after each time interval ($\grave{T}$), and the set of all but the last 12 time intervals ($\overline{\overline{T}}$) are defined (94).

The set of time intervals before the predicted failure time except the last MTTR time intervals is $T^{\dagger}$. If there is a prediction of failure within the time horizon, (95) ensures that an inspection is scheduled.

$$\sum_{t \in T} u_{j,t} \leq 1 \qquad \forall j \in J \quad (91)$$

$$\sum_{j \in J} u_{j,t} = 1 \qquad \forall t \in T \quad (92)$$

$$\left(1 - u_{j,t}\right) \geq m_{P1,t} + m_{P2,t} \qquad \forall j \in J, \forall t \in T \quad (93)$$

$$\sum_{\tau \in \grave{T}} u_{j,\tau} \leq 1 \qquad \forall t \in \overline{\overline{\overline{T}}} \quad (94)$$

$$\sum_{t \in T^{\dagger}} u_{P1,t} = 1 \qquad (95)$$

Resource constraints and variable bounds

The human, maintenance, and electricity resources used in relation to their requirements and capacities are computed via (96) - (103). Equations (102) and (103) describe the power consumption of the pumps [14]. Performance relationships for the turbines, condenser, and reboiler are obtained via high-fidelity simulation and regression and shown in (104)-(107). Bounds are shown in equations (108)-(113).

$$HRU_t = \sum_{j \in J} HRR_j^R m_{j,t} + \sum_{j \in J} HRR_j^I u_{j,t} \qquad \forall t \in T \quad (96)$$

$$HRU_t \leq HRC_t \qquad \forall t \in T \quad (97)$$

$$\mathrm{MRU_t} = \sum_{j \in J} \mathrm{MRR_j m_{j,t}} \qquad \forall t \in T \quad (98)$$

$$\mathrm{MRU_t} \leq \mathrm{MRC_t} \qquad \forall t \in T \quad (99)$$

$$\mathrm{ERU_t^{total}} = \mathrm{ERU_{P1,t}} + \mathrm{ERU_{P2,t}} - \mathrm{ERG_{B1,t}} - \mathrm{ERG_{B2,t}} \qquad \forall t \in T \quad (100)$$

$$\mathrm{ERU_t} \leq \mathrm{ERC} \qquad \forall t \in T \quad (101)$$

$$\mathrm{ERU_{P1,t}} = \frac{\mathrm{F_{s13,t}} \rho g H}{X \eta_{P1}} \qquad \forall t \in T \quad (102)$$

$$\mathrm{ERU_{P2,t}} = \frac{\mathrm{F_{s14,t}} \rho g H}{X * \eta_{P2}} \qquad \forall t \in T \quad (103)$$

$$\mathrm{ERG_{B1,t}} = \alpha_1 \mathrm{F_{s5,t}} + \alpha_2 \qquad \forall t \in T \quad (104)$$

$$\mathrm{ERG_{B2,t}} = \alpha_3 \mathrm{F_{s6,t}} + \alpha_4 \qquad \forall t \in T \quad (105)$$

$$\mathrm{Q_{E1,t}} = \alpha_5 \mathrm{R_t} + \alpha_6 \qquad \forall t \in T \quad (106)$$

$$\mathrm{Q_{E2,t}} = \alpha_7 \mathrm{F_{s2,t}} + \alpha_8 \qquad \forall t \in T \quad (107)$$

$$0 \leq \mathrm{F_{s,t}} \leq \mathrm{F^U} \qquad \forall s \in S, \forall t \in T \quad (108)$$

$$0 \leq \mathrm{F_{i,s,t}} \leq \mathrm{F^U} \qquad \forall s \in S, \forall t \in T \quad (109)$$

$$0 \leq \mathrm{T_{s3,t}} \leq \mathrm{T^U} \qquad \forall s \in S, \forall t \in T \quad (110)$$

$$\mathrm{R^L} \leq \mathrm{R_t} \leq \mathrm{R^U} \qquad \forall t \in T \quad (111)$$

$$0 \leq \mathrm{m_t^{TNT}} \leq \mathrm{m^{TNT,U}} \qquad \forall t \in T \quad (112)$$

$$0 \leq \mathrm{z_t^{TNT}} \leq \mathrm{z^{TNT,U}} \qquad \forall t \in T \quad (113)$$

5.4.3.4. Maintenance Scheduling and Process Optimization

The predicted failure time and probability of failure distribution were input into the maintenance scheduling and process optimization model. The model was optimized for multiple levels of the thresholds. This yielded a set of corresponding system effectiveness metrics. The full set of obtained set of solutions is shown in Figure 39. Each plotted point corresponds to a different combination of decision variables, and the decision maker can then select from the solutions to obtain an optimized trajectory of maintenance and process decisions.

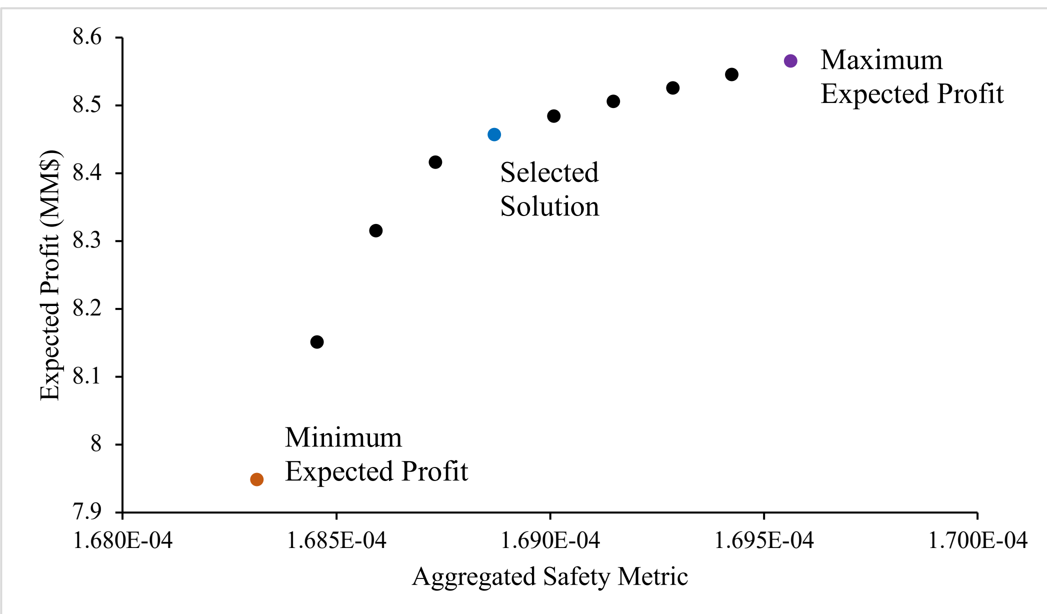


Figure 39: Case Study 2 - Pareto optimal maintenance and process solutions. Reprinted with permission from [52].

It is noted that the directionality of the aggregated safety metric is such that lower values are desired. It is further noted that the solution set is Pareto optimal with the epsilon-constraint for each of the solutions is active and no points being dominated.

The maximum expected profit case, a solution selected from qualitative assessment of the Pareto frontier, and the minimum expected profit case have been selected for further analysis. The optimized outlet flowrate of species B is presented in Figure 40 to illustrate process operating conditions for the cases.

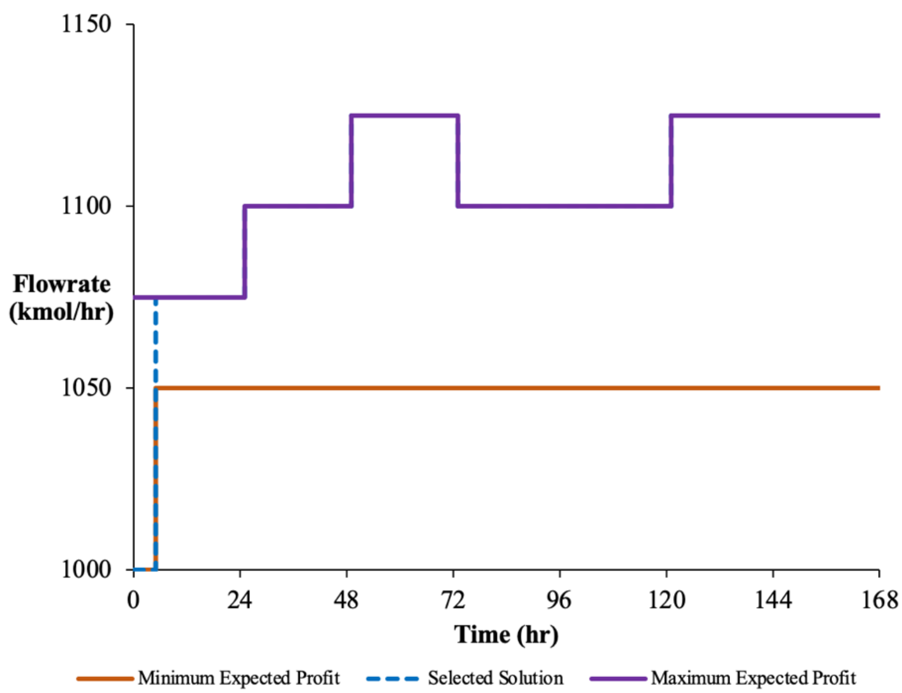


Figure 40: Optimized B flowrate. Reprinted with permission from [52].

It is observed that the maximum expected profit case has the highest flowrates over the time horizon and this is a result of the optimization recovering the upper production targets. The selected solution behaves similarly to the minimum expected profit case initially but then behaves similarly to the maximum expected profit case. The behavior of the selected solution is due to flowrates having been reduced sufficiently early in the scheduling horizon to allow for increased flowrates later in the horizon without adversely impacting the safety metric. The minimum expected profit case has the lowest flowrates over the time horizon with an initially reduced flowrate to the more costly and less energy-efficient secondary pump. It can be noted that a relatively modest change to production takes the system from the maximum expected profit solution to the selected solution, and that this change has a significant impact on the safety metric.

The maintenance schedules corresponding to the three selected cases are shown in Figure 41. It can be observed that in all three cases, the primary pump is repaired before the failure time, and that the other units are inspected at different spread out points in the horizon. It is noted that alternative inspection schedules can be obtained through the introduction of additional integer cuts if desired.

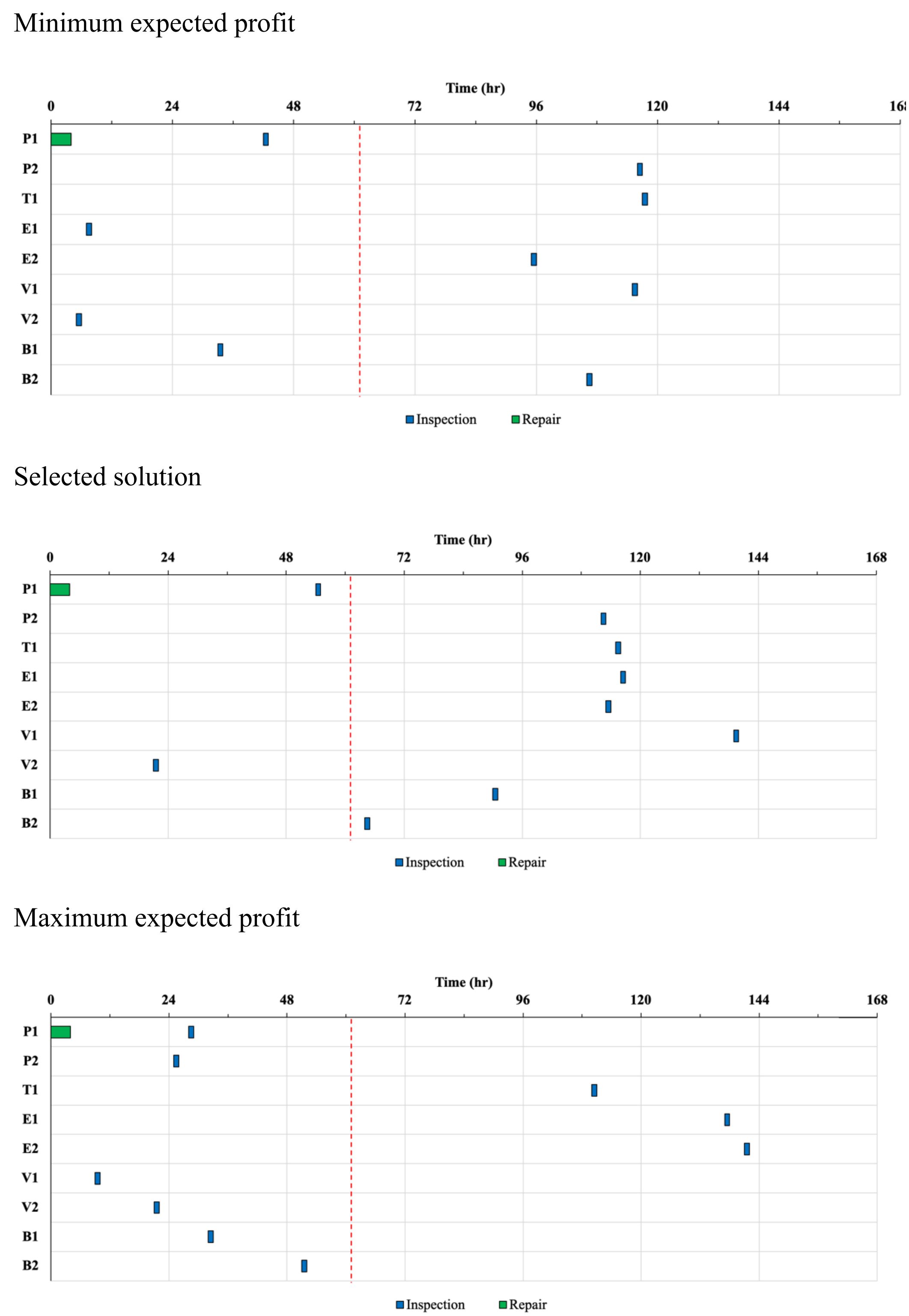


Figure 41: Optimized maintenance schedules. Reprinted with permission from [52].

5.4.3.5. Approach Comparison

This section contains a comparison between three approaches: corrective maintenance (CM), an example preventive maintenance (PM) approach, and the described prescriptive maintenance (PsM) approach.

In order to provide a common reference, it is assumed that maintenance on the primary pump has been conducted similarly until the start of the horizon and that the horizon occurs in the fourth quarter of the year, that the process operating conditions within the horizon would be the same, and that the equipment failure would occur at the predicted failure time. In the CM approach, the maintenance is done immediately after the failure time. In the PM approach, the maintenance time is determined from maintenance intervals calculated assuming as-good-as-new (AGAN) maintenance and the Weibull parameters reported in the supporting information. In the PsM approach, failure probability post-prescriptive maintenance is considered to be baseline. It is noted that more complex failure and repair models exist to capture specificities of processing systems, and that risk-based maintenance approaches could alternatively be used, however the specified methods have been used to avoid imparting additional complexity and lengthiness.

The metrics selected are overall equipment effectiveness (OEE) which would correspond to the availability over the horizon, and relative aggregated safety metric ($\widetilde{\Lambda}$) as defined in (114) and (115).

$$\mathrm{OEE_j} = \left(\frac{1}{168}\right)\sum_{t\in T} a_{j,t} \qquad \forall j \in J^P \quad (114)$$

$$\tilde{\Lambda} = \frac{\Lambda}{\Lambda^{CM}} \quad (115)$$

In all approaches, the relative aggregated safety metric is obtained from the predicted failure probability trajectory, and the failure probability post-failure is considered to be one. The results can be found in Figure 42 and Table 21.

It can be observed that corrective maintenance would potentially have resulted in a process safety incident and that preventive maintenance and prescriptive maintenance would have resulted in the process safety incident being avoided. It can also be observed that prescriptive maintenance has a better relative aggregated safety metric value. Given that preventive maintenance does not consider process information and prescriptive maintenance considers process information, this comparison illustrates the added value of considering process operating conditions in scheduling maintenance as prescriptive maintenance would accordingly have a higher expected profit than the other approaches. It is finally noted that different maintenance approaches may be more or less appropriate for different equipment in different services and processes.

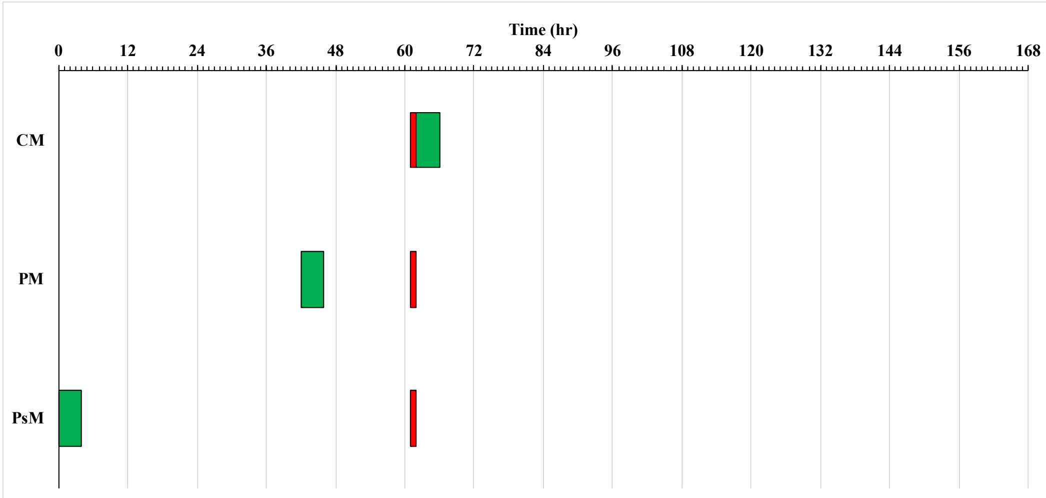


Figure 42: Maintenance schedules for different approaches. Reprinted with permission from [52].

Table 21: Comparison of different maintenance approaches. Reprinted from with permission [52].

Approach	**Incident**	**OEE**	$\widetilde{\boldsymbol{\Lambda}}$
Corrective	Yes	36.3%	1
Preventive	No	97.6%	0.014
Prescriptive	No	97.6%	0.001

5.5. Conclusions

Optimized resource allocation, process optimization, and scheduling can help improve system effectiveness and system resilience. This paper contributes a framework that combines process safety, machine learning for failure prediction, and mathematical optimization. The framework was illustrated through a motivating example and a case study, and used for integrated maintenance scheduling and process optimization.

Equipment mechanical failure prediction was done using ensembles of support vector machine classifiers. The classifiers were evaluated on validation data not used to train the models. The individual classifiers had an overall F1-score of 95.9% and an overall accuracy of 95.7%. The ensemble classifiers had a overall F1-score of 98.7% and an overall accuracy of 98.7%. It is noted that different model performance metric values can be expected for different input historical data. It was seen here that the ensemble classifiers performed better than the individual classifiers.

The ensemble classifiers were used to predict a failure probability trajectory and failure time. The failure prediction outputs were fed as parameters to a multi-objective mixed-integer nonlinear programming model to determine sets of process and maintenance decisions that simultaneously optimized profit and a safety metric.

Future work will be focused on weighted tuning via cost-sensitive support vector machine classification to improve model performance, comparing the performance of the approach on multiple data sets, incremental learning, comparing the approach to risk-based maintenance, and on safety-aware maintenance-aware fault-aware multiparametric model predictive control to link fault detection with maintenance scheduling and control.

The developed framework is process-agnostic as well as safety metric-agnostic, and can be adapted for use with other failure prediction, safety quantification, and optimization methods.

6. DATA-DRIVEN PRESCRIPTIVE MAINTENANCE TOWARD FAULT-TOLERANT MULTI-PARAMETRIC CONTROL*

6.1. Summary

Prescriptive maintenance can improve system effectiveness and system safety via integrated production and maintenance optimization. However due to system disruptions there is potential for abnormal operations and an undesirable increased occurrence of process safety incidents. This research provides a multi-parametric-based framework for safety-aware maintenance-aware and disruption-aware process control. It leverages ensemble classification via machine learning classifiers for fault detection, mixed-integer nonlinear programming for integrated safety-aware production and maintenance scheduling, as well as hybrid multi-parametric model predictive control for fault-tolerant setpoint tracking. The results show that the ensemble classifier outperforms the individual classifiers in terms of fault detection accuracy, sensitivity, and specificity. Furthermore, it is seen that the developed controllers are able to reconfigure the control actions based on process disruption information. The framework is illustrated with a chemical complex system, and a cooling water system. The approach can be used to help improve the safety and productivity of industrial processes.

---

* This chapter was submitted as Gordon, C. A. K.; Pistikopoulos, E. N. Data-Driven Prescriptive Maintenance toward Fault-Tolerant Multi-Parametric Control. AIChE Journal. Copyright American Institute of Chemical Engineers.

6.2. Introduction

Prescriptive maintenance seeks to determine the set of integrated maintenance and production decisions that improve the effectiveness of process systems. These decisions can be complex as they: interact, impinge upon multiple time scales, and affect the level of system safety.

Disruptions pose challenges to system effectiveness and safety. From a process monitoring perspective, these disruptions can be classified as: (1) faults, which are deviations in system parameters from nominal values and can be countered via process actions; (2) failures, which are severe functionality interruptions that can be countered by maintenance actions but not by process actions; and (3) disturbances, which are uncontrolled system inputs.[281] These disruptions have the potential to lead to abnormal operations and an undesirable increased occurrence of process safety incidents. It is thus of great interest to leverage state-of-the art techniques to support decision-making.

This research draws upon a number of research areas to tackle the challenges associated with process disruptions. Machine learning is a field of artificial intelligence that can help account for the complexity of process disruptions through data-centric and methodological inference of relationships between system variables.[19, 281] Mathematical optimization is used to tackle the associated problem of constrained resource allocation through its ability to account for nonlinear and discrete system phenomena via rigorous algorithms.[25] Multi-parametric model predictive control (mpMPC) is leveraged to provide rapid controller response through its shifting of the computational optimization burden offline to yield explicit optimal control laws as a function of system parameters.[352] A summary of the related literature is provided in Table 22.

This research presents a framework for prescriptive maintenance. The framework involves: equipment failure prediction using machine learning, maintenance and production scheduling with safety constraints using mathematical optimization, high-fidelity dynamic simulation, as well as multi-parametric model predictive control. The framework is applied to a chemical complex case study as well as a cooling system case study. It is stressed that the framework considers the two time scales of scheduling and control as well as both faults and failures.

This research builds upon previous efforts and develops a methodology which includes the consideration of maintenance for multi-parametric model predictive control. Key features of the proposed methodology include development of: a diverse ensemble classifier for fault detection consisting of an artificial neural network, decision tree, and support vector machine model; constrained mixed-integer nonlinear programming to maximize profit and minimize cost; as well as fault-tolerant multi-parametric model predictive control towards maintaining setpoint tracking in the presence of system disruptions.

Table 22: Indicative summary of related previous work

Reference(s)	Description
	Fault Detection
[353]	Principal component analysis for fault detection and discriminant methods for fault diagnosis
[354]	Feature extraction and random forest classification
[74]	Feature selection and one-class support vector machine classification
[115]	Outlier detection via Gaussian process regression and classification
[81, 267, 346]	Simultaneous fault detection and diagnosis using support vector machines
	Process and Maintenance Scheduling
[145]	Overall profitability maximization of multipurpose equipment
[204]	System effectiveness optimization considering environmental impact
[143]	Short-term preventive maintenance scheduling using mixed-integer linear programming
[118]	Robust mixed-integer linear programming involving equipment condition degradation modeling
[52]	Multiobjective profit and safety optimization and ensemble support vector classification failure prediction
	Fault-aware Control
[267]	Multi-parametric model predictive control with estimated fault magnitudes as parameters
[254]	Post-sensor fault measurement correction with process control
[239]	Fault magnitude quantification via parameter estimation
[253]	Reconfiguration of the model predictive control objective function coefficient matrix
[232]	Disturbance-aware model predictive control and observer-based fault detection
	Hybrid Model Predictive Control
[355]	Modeling and control of mixed logical dynamical systems
[356]	Branch and bound algorithm for multi-parametric mixed-integer quadratic programming problems
[357]	Online model predictive control considering a piecewise-defined state-to-input matrix and reduced number of state transitions
[358-361]	Hybrid multi-parametric model predictive control algorithms and applications
[289]	Online model predictive control using a tree traversal algorithm

6.2.1. Problem Statement

This research seeks to address the problem defined by the following components:

Generalized System

A process network involving species $i \in I$, equipment $j \in J$, process streams $s \in S$, utilities $u \in U$, scheduling time intervals $t^S \in T^S$, and control time intervals $t^C \in T^C$.

Objectives

- Maximize system effectiveness
- Setpoint tracking

Given

- Process network design
- High-fidelity dynamical model
- Equipment condition, failure, and error data
- Production, atmospheric, maintenance, and economic data
- Species supply and demand parameters
- Safe operating limits
- Process deviation measurements

Determine

- Failure prediction
- Production and maintenance schedule
- Fault existence
- Sequence of optimal control actions

6.3. Methodology

6.3.1. mpSAMADA Framework

This research presents as well as implements a multi-parametric-based safety-aware, maintenance-aware, and disruption-aware (mpSAMADA) framework for prescriptive maintenance. The framework spans a number of different aspects as shown in Figure 43.

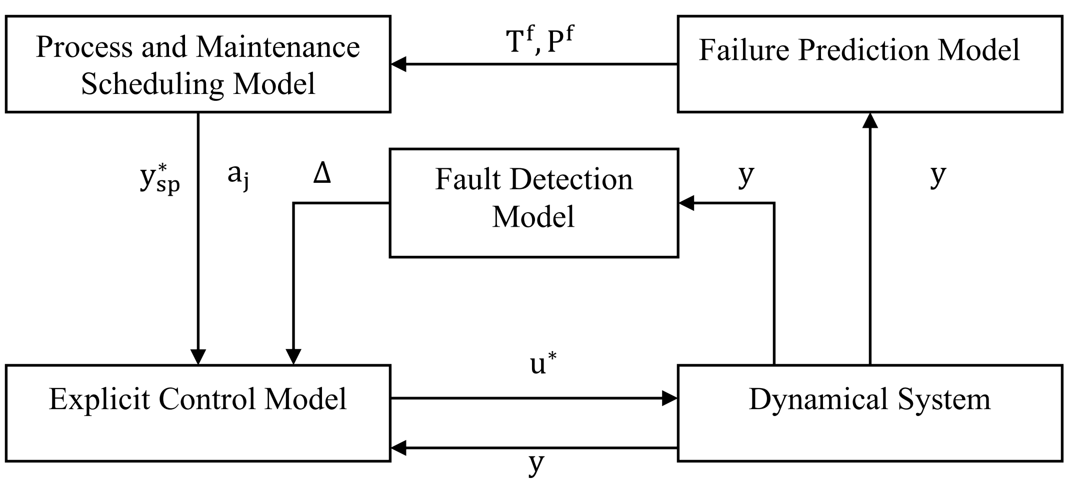


Figure 43: mpSAMADA framework

The scheduling model is based on mathematical programming. It is safety-aware via inclusion of process safety constraints. It is maintenance-aware via inclusion of maintenance constraints. It is disruption-aware via use of the time (T_f) and probability trajectory (P_f) of failure for scheduling.

The control model is based on multi-parametric model predictive control. It is developed using a surrogate model created from dynamic simulation measurements (y). It is safety-aware via constraints on system states, inputs, and input changes. It is maintenance-aware via use of discrete-valued equipment availabilities (a_j) as state-transition indicators. The corresponding continuous-valued scheduled production decisions are used as controller setpoints (y_{sp}^*). It is disruption-aware via consideration of a fault parameter (Δ) that captures a detected fault magnitude.

The key outputs of the mpSAMADA framework are a production schedule, a maintenance schedule, and control actions (u^*).

The key aspects of the overall methodology are summarized in Table 23 and this chapter proceeds to describe each of them in more detail.

Table 23: Summary of methodology

#	**Aspect**	**Input**	**Output**
1	Failure Prediction	Historical data	Failure probability trajectory Failure time
2	Scheduling	Failure probability trajectory Failure time System parameters	Continuous-valued production setpoints Discrete-valued equipment availabilities
3	Fault Detection	Process measurements	Fault parameter
4	Control	Surrogate state-space model Continuous-valued production setpoints Discrete-valued equipment availabilities Fault parameter	Explicit hybrid control laws

6.3.2. Failure Prediction and Scheduling

The failure prediction and scheduling models follow a similar paradigm to that of the authors' previous work to which researchers interested in implementing are kindly referred.[52] This subsection summarizes the essential aspects for brevity and links them to the other framework components. It is noted that the scheduling and control problems are treated separately here and that it is assumed that transitions to new operating points are mostly resolved within the scheduling time discretization. It is further noted that work related to the integrated scheduling and control problem has been done for systems in which this assumption does not hold.[230, 237, 362]

The objective of failure prediction is to estimate when a piece of equipment will likely fail. The authors used five key steps to predict failure in their previous work: (1) preprocessing of diverse system data, involving statistical feature generation and Z-score normalization; (2) feature selection, involving recursive feature elimination; (3) splitting, to divide data into training and test sets; (4) model creation, using multiple nonlinear support vector classifiers; and (5) prediction, consolidating individual support vector machine models into ensemble models over rolling prediction horizons.[52] It is noted that the mpSAMADA framework is flexible for use with alternative failure prediction methods. The present work uses a two-parameter sigmoid function to model failure probability and illustrate the framework. The outputs of the failure prediction are: (1) the estimated time of failure, and (2) a vector containing the predicted probabilities of failure.

The scheduling model leverages the failure prediction model outputs to optimize maintenance and production. This is done by formulating the problem as a constrained mixed-integer nonlinear programming model subject to production, maintenance, availability, and safety constraints. The scheduling model is solved and then used to inform the optimal control model.

6.3.3. Fault Detection

The fault detection model methodology consists of two phases: (1) an offline phase, and (2) an online phase.

An overview of the offline phase is provided in Figure 44. Historical training and test data are imported. The rows of the data are termed samples, and the columns of the data are termed features. The data is labelled and consists of both normal and faulty samples. The data is first preprocessed via Z-transformation. Wrapper feature selection is then performed on the transformed data via recursive feature elimination. A random forest classification algorithm is leveraged for this due to its intrinsic ability to rank features based upon their importance. The selected features are then used to filter the data and provide a smaller data set for faster and more accurate training.

Data-driven model creation then proceeds. Three classifiers are created: (1) an artificial neural network (ANN) model; (2) a decision tree (DT) model; and (3) a cost-sensitive C-parametrized support vector machine (SVM) model. Background information about these models can be found in another study [20].

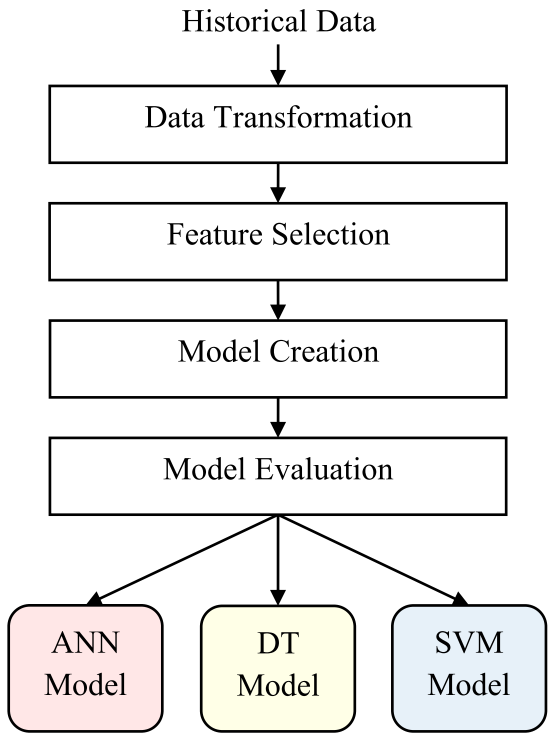


Figure 44: Overview of fault detection methodology – Offline phase

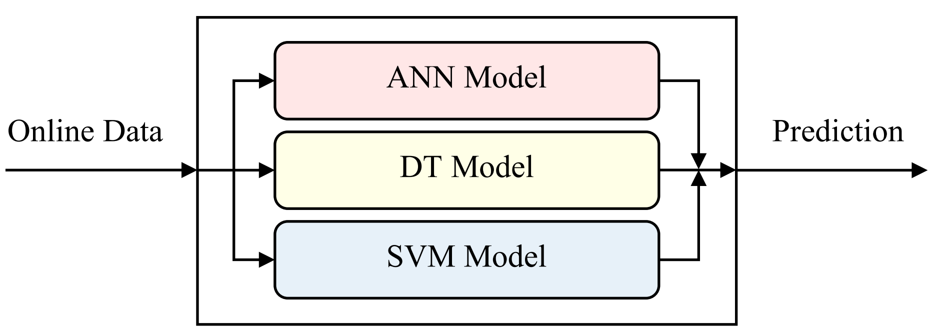


Figure 45: Overview of fault detection methodology – Online phase

One distinguishing feature of the present research is the combination of these multiple different models into ensemble for fault detection. This has the advantage of improving prediction accuracy due to being able to average the votes of individual classifiers, provide a better approximation to the phenomena being modeled, and model a more diverse range of phenomena.[363]

An overview of the online phase is provided in Figure 45. The ensemble model makes a determination as to whether or not a sample of online data corresponds to a fault based upon simple majority voting. The output of the fault detection methodology is thus an ensemble fault detection model that predicts fault existence if two out of the three constituent individual classifiers each label a given sample as faulty.

6.3.4. Explicit Control

An explicit control model is developed for each major piece of equipment. The following discussion touches upon how the present research addresses disruptions and hybrid explicit controller creation.

The control methodology accounts for both failures and faults. Predicted equipment failures directly affect production and maintenance scheduling which indirectly affects control by influencing set points and state transitions. Predicted faults directly affect control through the use of a fault parameter (Δ). This fault parameter is comprised of: (1) fault magnitude (δ), the deviation of a process measurement from its nominal value, and (2) fault existence ($y^f \in 0,1$), which is obtained from the fault detection model. It is noted that this research focuses on process faults as well as actuator faults but does not consider sensor faults. An assumption is made here that after fault detection, either a sensor fault magnitude estimator is available or that sensor measurements can be trusted to provide a measure of the fault magnitude. The functional form of the fault parameter (Δ) is shown in (116).

$$\Delta = \delta y^f \tag{116}$$

The fault parameter thus takes on two values: (1) the fault magnitude, if a faulty situation is predicted, or (2) zero, if a non-faulty situation is predicted. From the perspective of process control, this fault parameter is then used as a disturbance magnitude.

The control methodology continues with the use of multi-parametric model predictive control to build hybrid explicit controllers. This is done using the PARametric Optimisation and Control (PAROC) framework for optimal and explicit control of dynamic processes subject to uncertainty and varying parameters.[352]. This framework allows the computational burden of determining optimal model-based control laws to be transferred offline, and reduces the online computational effort of model predictive control to point location and function evaluation. The steps of the PAROC framework are summarized in Figure 46 and then described.

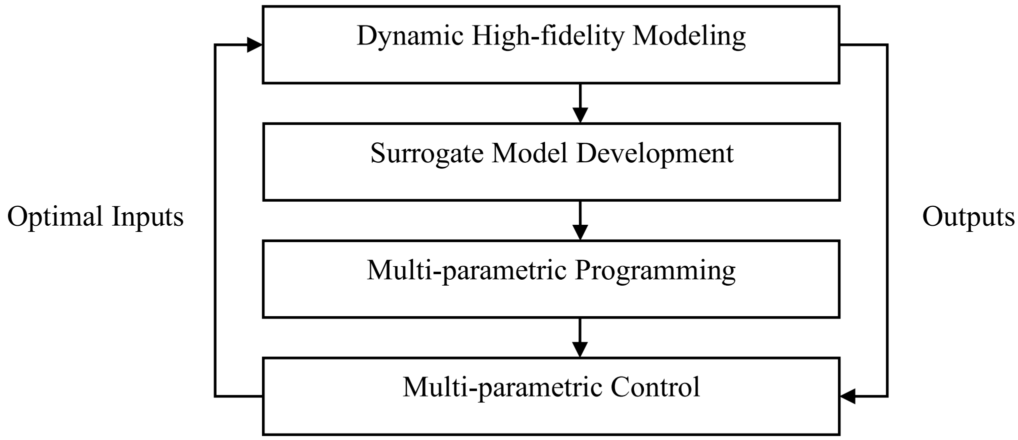


Figure 46: PARametric Optimisation and Control (PAROC) framework

Step 1: involves dynamic high-fidelity process modeling. This leverages a system of differential-algebraic equations to capture system phenomena.

Step 2: involves surrogate model development. This involves the development of reduced-order models that are more tractable for control applications. It is noted that the PAROC framework extends to systems with discrete events such as equipment becoming unavailable due to maintenance being performed. These events can lead to system state transitions and different regimes of system dynamics $k \in K$. The output of the second step in this context is a piecewise affine (PWA) surrogate model in which states (x_t), inputs (u_t), disturbances (d_t), and outputs (y_t) have regime-dependent state-space matrices (117).

$$x_{t+1} = A_k x_t + B_k u_t + C_k d_t \tag{117}$$

$$y_t = D_k x_t + E_k u_k$$

Step 3: involves multi-parametric programming. This involves using the surrogate model together with offline solution of the model predictive control problem. The output of this step is a control map. Each region of the control map contains an explicit control law that maps system measurements and the fault parameter to optimal control actions.

Step 4: involves closed-loop validation. This involves the use of the developed controller with the high-fidelity model to assess its performance.

It is noted in passing that the mpSAMADA framework is in line with recent trends towards smart manufacturing, digitalization, and artificial intelligence. Of particular note is the ability to embed the explicit control laws resulting from the multi-parametric model predictive control on a chip which is of interest for next-generation edge computing and rapid control actions.

The paper then proceeds to apply the approach on two case studies.

6.4. Results

6.4.1. Overview of Model Implementation

This research used a number of different software environments. The failure prediction model and outputs were generated in MATLAB R2020a. The maintenance and production scheduling was carried out in GAMS 27.1.0 using BARON.[364] The fault detection was done in R 3.5.1. The high fidelity dynamic models were implemented in gPROMS ModelBuilder 6.0. MATLAB R2020a was used to build the surrogate state-space models using the System Identification Toolbox as well as to build the multi-parametric model predictive control models using the POP Toolbox.[365] The cross-validation was done by integrating gPROMS and MATLAB using gO:MATLAB. Both case studies were implemented in the same software environments.

6.4.2. Case Study 1 – Chemical Complex

6.4.2.1. Description

The system used for the first case study is a chemical complex and was taken from Vassiliadis and Pistikopoulos.[7] The objective of the first case study is to illustrate how the different components of the framework link. In this illustrating example, the failure prediction and fault detection are effectively treated as given inputs and the focus is on the scheduling and control aspects of the framework. It is noted that this example involves multiple processing routes as well as multiple units which enables elucidation of maintenance and production interactions.

The system is depicted in Figure 47 and its scheduling parameters are provided in the Appendix. The overall objective of the system is to convert species A to species C to satisfy downstream demand. Feed is supplied to reactors one, two and three in the top branch and to reactor four in the bottom branch. In the top branch, reactors one and two convert A to an intermediate species B which is then converted to species C by reactor three. In the bottom branch, reactor four converts species A to species C directly.

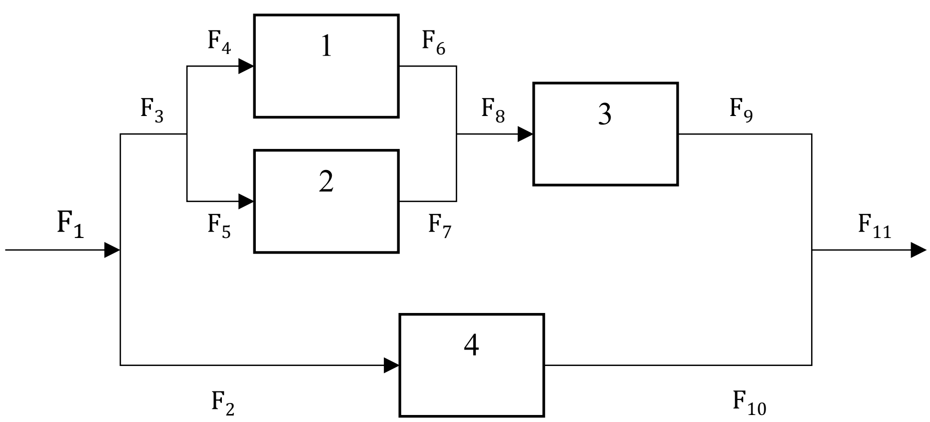


Figure 47: Case Study 1 – Chemical complex system

6.4.2.2. Maintenance and Production Scheduling

The problem statement for the process optimization and maintenance scheduling model is provided as follows. The objective is to maximize the system effectiveness metric of expected profit. The scheduling horizon is one day. It is assumed that only one type of maintenance is performed, mean time to repair (MTTR) is fixed, there are no resource constraints on maintenance, and that maintenance repairs equipment to an as-good-as-new (AGAN) condition. The inputs that are given include the design of the process network, cost parameters, and failure information. The key binary variables are the availability of the first reactor unit and whether or not to maintain it in a given time interval. The key continuous variables considered are flowrates (F). The model formulation involves four equipment $j \in J$, eleven streams $s \in S$, twenty-four hourly time intervals $t \in T$, and an aggregated utility $u \in U$.

The expected profit objective function (Φ) is shown in (118). It consists of product revenue, feed cost, maintenance cost, and utility cost terms as well as the probability of the system being in a non-failure state which is taken to be the system reliability (R_t^{sys}). The objective function is subject to process constraints, availability constraints, and maintenance constraints.

$$\max \Phi = \sum_{t \in T} R_t^{sys} \left[C^R F_{11,t} - C^C F_{1,t} - \sum_{j \in J} C_j^M m_{t,j} - \sum_{j \in J} \sum_{s \in S^j} C_j^U F_{s,t} \right] \qquad (118)$$

The process constraints are taken from another study. [7]

$$F_{1,t} = F_{2,t} + F_{3,t} \qquad \forall t \in T \qquad (119)$$

$$F_{3,t} = F_{4,t} + F_{5,t} \qquad \forall t \in T \qquad (120)$$

$$F_{6,t} = \alpha_1 F_{4,t} \qquad \forall t \in T \qquad (121)$$

$$F_{7,t} = \alpha_2 F_{5,t} \qquad \forall t \in T \qquad (122)$$

$$F_{6,t} + F_{7,t} = F_{8,t} \qquad \forall t \in T \qquad (123)$$

$$F_{9,t} = \alpha_3 F_{8,t} \qquad \forall t \in T \qquad (124)$$

$$F_{10,t} = \alpha_4 F_{2,t} \qquad \forall t \in T \qquad (125)$$

$$F_{11,t} = F_{9,t} + F_{10,t} \qquad \forall t \in T \qquad (126)$$

$$F^{D} \leq F_{1,t} \leq F^{S} \qquad \forall t \in T \qquad (127)$$

The availability ($a_{j,t}$) constraints prevent flow to the reactors if they are unavailable due to being maintained ($m_{t,j}$).

$$F_{4,t} \leq F^{U}_{R1} a_{1,t} \qquad \forall t \in T \qquad (128)$$

$$F_{5,t} \leq F^{U}_{R2} a_{2,t} \qquad \forall t \in T \qquad (129)$$

$$F_{8,t} \leq F^{U}_{R3} a_{3,t} \qquad \forall t \in T \qquad (130)$$

$$F_{2,t} \leq F^{U}_{R4} a_{4,t} \qquad \forall t \in T \qquad (131)$$

$$1 - a_{j,t} \geq m_{j,t} \qquad \forall j \in J, \forall t \in T \qquad (132)$$

The maintenance constraints impact maintenance and availability. A failure time prediction of 16 hr for reactor one is fed as an input parameter to the maintenance constraints. It is assumed that this failure does not result in loss of containment. Maintenance is constrained to start once before the failure time by (133) where the time intervals before the predicted failure time are denoted T^1.

$$\sum_{t \in T^1} m_{,t}^{start} = 1 \tag{133}$$

Maintenance is further constrained to: not occur simultaneously on reactors one and two by (134) for safety, as well as to continue contiguously once started for only the repair time by (135) and (136). Constraints (137) - (139) help indicate if prior maintenance was done in the time horizon. A number of subsets are defined: the equipment maintenance list J^1 consisting of the first reactor, MTTR time intervals after and including each possible m start time (T^2), all time intervals except the last (MTTR - 1) time intervals (T^3), all time intervals except the last time interval (T^4), and sets of time intervals before each given time interval (T^5).

$$m_{R1,t} + m_{R2,t} \leq 1 \qquad \forall t \in T \tag{134}$$

$$\sum_{\tau \in T^2} m_{j,\tau} \geq MTTR_j m_{j,t}^{start} \qquad t \in T^3 \ \forall j \in J^1 \tag{135}$$

$$\sum_{t \in T} m_{j,t} \leq MTTR_j \qquad t \in T \ \forall j \in J^1 \tag{136}$$

$$m_{j,t+1}^{prior} \geq m_{j,t}^{start} \qquad \forall t \in T^4 \forall j \in J^1 \quad (137)$$

$$m_{j,t+1}^{prior} \geq m_{j,t}^{prior} \qquad \forall t \in T^4 \forall j \in J^1 \quad (138)$$

$$\sum_{\tau \in T_t^5} m_{j,\tau}^{start} \geq m_{j,t+1}^{prior} \qquad t \in T^4 \ \forall j \in J^1 \quad (139)$$

Maintenance is linked to component reliability, system reliability, as well as expected profit by safety constraints (140) - (142). A predicted failure probability trajectory for reactor one is input to the scheduling model as a corresponding predicted reliability ($R_{1,t}^{pred}$) defined by parameters (λ_1 and λ_2). It is assumed that the other reactors have been outfitted with predictive maintenance (PdM) systems which returned constant reliabilities over the scheduling horizon of one day. It is thus noted that system reliability here reduces to an affine function of the reliability of reactor ($R_{1,t}$).

$$R_{1,t}^{pred} = \frac{1}{1 + e^{-\lambda_1 (t - \lambda_2)}} \qquad \forall t \in T \quad (140)$$

$$R_{1,t} = R_{1,t}^{pred}\left(1 - m_{1,t}^{prior}\right) + (1) m_{1,t}^{prior} \qquad \forall t \in T^4 \quad (141)$$

$$\begin{aligned} R_t^{sys} = {} & R_{1,t}R_3 + R_2R_3 - R_{1,t}R_2R_3 + R_4 - R_{1,t}R_3R_4 \\ & - R_2R_3R_4 + R_{1,t}R_2R_3R_4 \end{aligned} \qquad \forall t \in T \quad (142)$$

The scheduling model has 457 continuous variables, 311 binary variables, as well as 733 constraints. It is solved and the results are summarized in Figure 48.

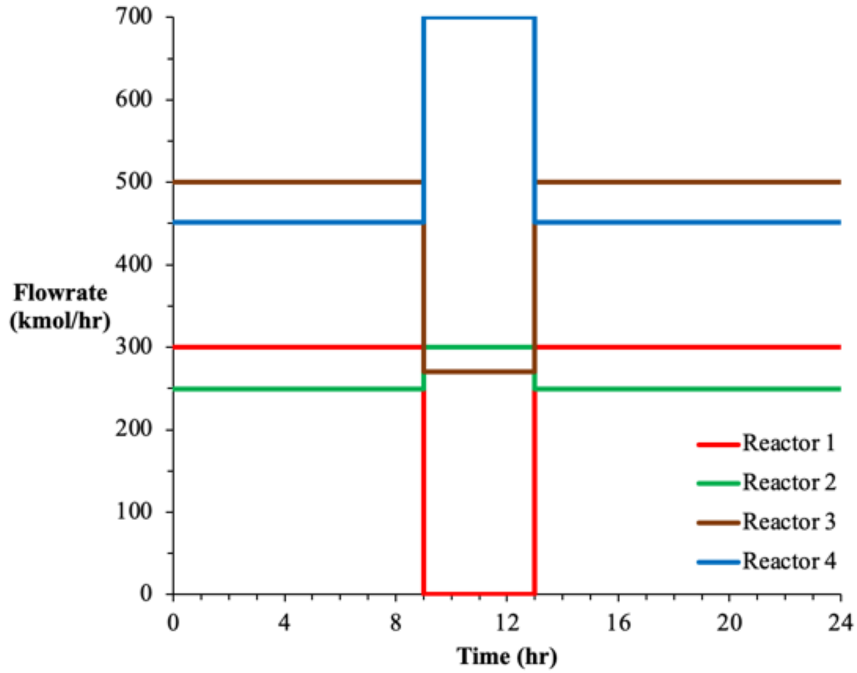


Figure 48: Case Study 1 – Production trajectories

It can be seen that before maintenance the production is optimized by using both the top branch and the bottom branch. It is noted that reactor four has a higher capacity, higher utility cost, and lower conversion than reactors one and two combined. Consequently, it is seen that more feed is provided to reactors one and two than reactor four to increase expected profit. It is observed that reactor one is maintained before the failure time. The system reconfigures to a state in which there is a cessation of flow to reactor one, reactor one is made unavailable, and the load of the other reactors is adjusted. Specifically during maintenance, reactor two takes on the maximum additional feed possible and reactor four has an increased inlet flowrate. This is reflective of the top branch having a lower utility cost and a slightly higher overall conversion than the bottom branch. After maintenance, the system returns to its previous regime. The scheduling results are then used to inform the control of the system.

6.4.2.3. Explicit Control

The results presented here correspond to the system regime in which reactor one is unavailable and the other reactors are available. The scope of the subsequent discussion is for reactor two.

The outputs are concentration (C_A), and reactor temperature (T). The manipulated input is cooling jacket water temperature (T_c). The unmanipulated input or disturbance is cooling water flowrate (m_c). The fault parameter is taken as a given input corresponding to a 5% decrease in the cooling water flowrate. The control objective is to maintain conversion near 90% which corresponds to a concentration setpoint of 1 mol/L. The mpMPC design follows the PAROC framework steps.

Step 1: High-fidelity dynamic modeling

The reactor model was adapted from another study,[241] and the parameters used are provided in the Supporting Information. It is assumed that all components are in liquid phase, there is perfect mixing, and that all states are measurable.

$$\frac{dC_A}{dt} = \frac{m}{\rho V}\left(C_{A,0} - C_A\right) - k_0 e^{-\frac{E_a}{RT}} C_A \tag{143}$$

$$\frac{dT}{dt} = \frac{mC_p(T_0 - T) + V\Delta H_{rxn} k_0 e^{-\frac{E_a}{RT}} C_A + UAm_c(T_c - T)}{\rho V C_p} \tag{144}$$

Step 2: Model approximation

The surrogate state-space model was developed from input-output data. This was generated by initializing the high-fidelity model at steady-state, perturbing the cooling temperature by ± 5 °C, and then perturbing the cooling flowrate by ± 1 kg/s at a sample time of 1 s. Model approximation was done in MATLAB using the System Identification Toolbox to construct a surrogate state-space model. The fit of the surrogate model to the data was 83.64% for concentration and 97.75% for temperature as shown in the Supporting Information.

The identified state-space model took the form of (145). The state-space model contains pseudo-states (x_t), cooling water temperature as an input (u_t), as well as cooling flowrate as a disturbance (d_t). It is stressed that while the pseudo-states do not correspond directly to the physical states, the outputs (y_t) of the surrogate model correspond to the physical outputs.

$$x_{t+1} = Ax_t + Bu_t + Cd_t \tag{145}$$

$$y_t = Dx_t$$

Step 3: Multi-parametric programming

The identified state-space model was then used to build a mpMPC controller in MATLAB. The control model and tuning parameters can be found in Appendix C. The parameter (θ) vector is shown in (146) and consists of the pseudo-states, the magnitude of the cooling water flowrate disturbance, and the conversion setpoint.

$$\theta := [\theta_1, \theta_2, \theta_3, \theta_4] = \left[x_{1_{t=0}}, x_{2_{t=0}}, d_{t=0}, y_t^{sp}\right] \quad (146)$$

The control model was optimized using the POP toolbox to yield 12 critical regions over the entire parameter space. A slice of the control map for certain parameters fixed at nominal values is shown in Figure 49. It is noted that each critical region corresponds to an explicit control law that links the jacket temperature to the parameters.

Step 4: Closed-loop validation

The controller was then validated against the high-fidelity model. As shown in Figure 50, it can be seen that although there is some variation concentration, the controller is able to maintain the conversion near the setpoint. It is further noted that the controller is able to safely maintain the reactor temperature despite the cooling flowrate disruption.

Online application of the controller involves simply locating points in the control map and then evaluating the control laws to get the control actions.

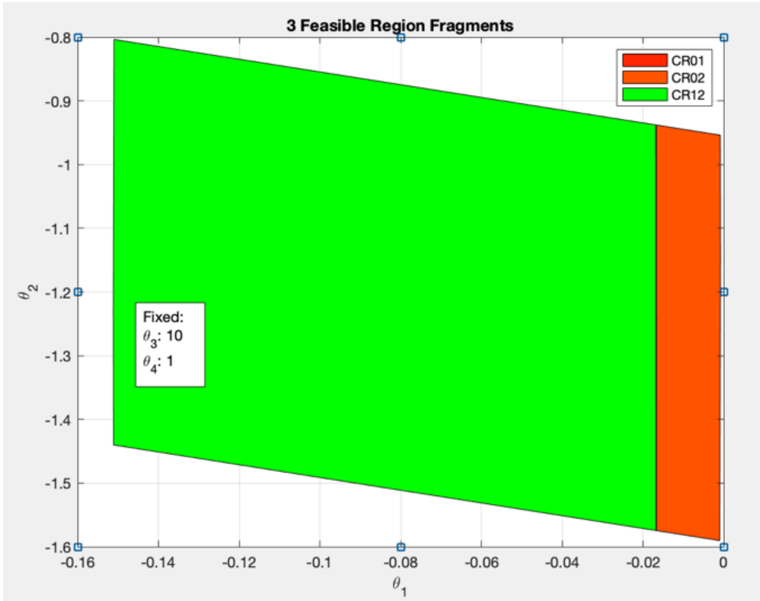


Figure 49: Case Study 1 - Control map

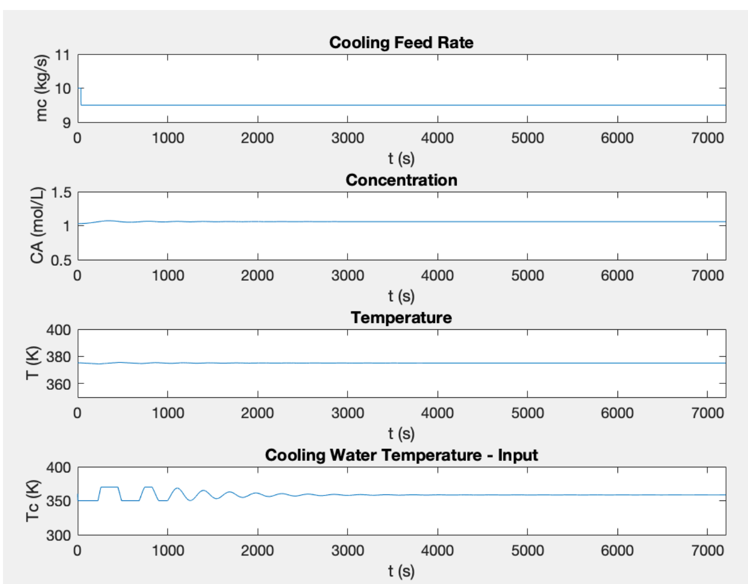


Figure 50: Case Study 1 - Closed-loop validation

6.4.3. Case Study 2 – Cooling System

6.4.3.1. Description

A cooling system was used for the second case study. It adapts fault information, [242] system structure, [9] and constraints [366] from other work. The objective of the second case study is to illustrate the fault detection component of the framework in greater depth. In this example, the failure prediction is treated as a given input. The focus here is on the fault detection and control aspects of the framework. It is noted that the process data used in example involves a large number of features that exhibit high variability which render fault detection non-trivial. The system is depicted in Figure 51 and its scheduling parameters are shown in the Supporting Information.

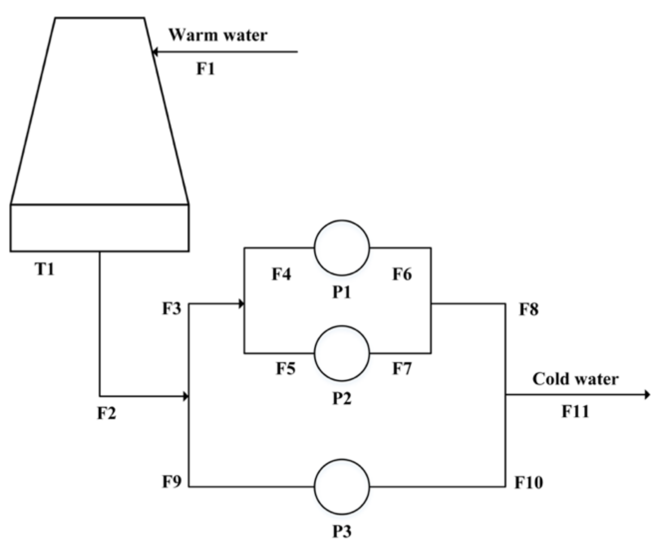


Figure 51: Case Study 2 – Cooling system

The overall objective of the system is to provide an fixed and uninterrupted supply of cooling water for the reactor in the Tennessee Eastman Process (TEP).[242] Warm recycled water is sprayed onto the film fills of a mechanical forced draft cooling tower to bring it into contact with a fan-induced counterflow air steam to reduce the temperature to process requirements. The cooled water is accumulated in a basin and then returned to the reactor by a pump network.

6.4.3.2. Maintenance and Process Scheduling

The problem statement for the process scheduling and maintenance scheduling model is provided as follows. The objective is to minimize expected cost. The scheduling horizon is one day, with an hourly time discretization. The model formulation for the process and maintenance scheduling proceeds similarly to the first case study and can be found in the Supporting Information. Similarly, a failure time prediction of 8 hr for pump one and corresponding failure probability trajectory are input to the scheduling model as parameters. The key binary variables are the availabilities of the first pump and whether or not to maintain it in a given time interval. The key continuous variables considered are flowrates. The scheduling model has a combined total of 1201 continuous variables, 263 binary variables, as well as 1695 constraints. The optimization results are summarized in Figure 52.

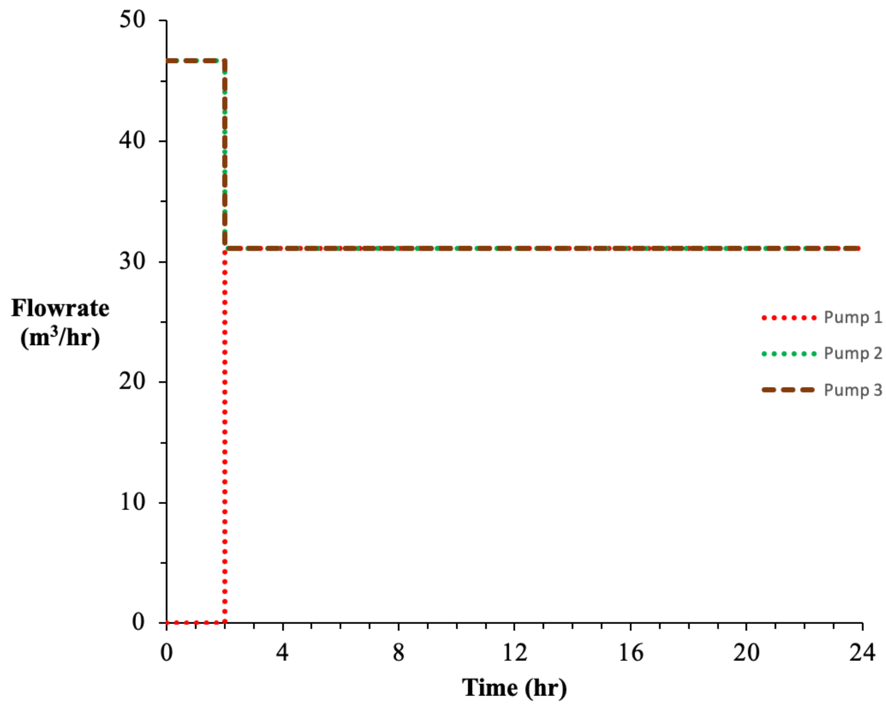


Figure 52: Case Study 2 – Process trajectories

The optimization results reflect the maintenance and process decisions that minimize the overall expected cost of the cooling process. These decisions are embedded within the pump flowrate trajectories. It can be seen that maintenance is performed on the first pump early on in the time horizon. During the repair time, the first pump is made unavailable. This leads to no flowrate through the first pump and the other two pumps taking on the load and experiencing higher flowrates. It is noted that having three parallel pumps operating at reduced capacity helps avoid single-point failures that could shut down entire processes.

The system experiences a regime transition in moving from running two pumps to running three pumps after maintenance is completed. Operating the other two pumps at higher flowrates corresponds to operating them away from their best-efficiency points (BEP). This results in a reduced pump energy efficiency and higher energy cost. As such after maintenance the load is redistributed so that the three pumps share the flow.

It is noted in passing that from a process safety perspective, excessive operation of pumps away from their BEP can lead to an increased probability of failure. It is further noted that operating two pumps imparts less process flexibility than operating three pumps due to the negative impact on the downstream process if an additional pump were to experience failure within the maintenance window. It can finally be observed that the total flowrate of cooled water remains constant over the time horizon as is desired. This however is not always the case due to faults which can result in the supply of cold utility being disrupted.

Production setpoints and availabilities are used to inform the control of the system.

6.4.3.3. Fault Detection

6.4.3.3.1. Dataset Description

The process disruption considered here is a cooling water valve sticking. The data used for fault detection was data corresponding to the Tennessee Eastman Process.[242] The data used consisted of three datasets: a training set of 980 samples, comprising 500 normal and 480 faulty samples; a test set of 960 samples, comprising 480 normal and 480 faulty samples; and an 'online' set sampled from the test set, comprising 1 faulty sample. These datasets were used as follows: the training set was used to create the models, the test set was not shown to the models but rather used to evaluate the models, and the 'online' set was used to make a fault prediction. The 52 features of the data are listed in the Supporting Information.

6.4.3.3.2. Feature Selection

Feature selection assessed the performance of progressively smaller subsets of features as shown in Figure 53 and Figure 54. It can be observed that using more features does not necessarily correspond to increased model performance and that a comparable or even better level of performance can be achieved with fewer features here. It is noted that fewer features desirable for quicker training, as well as useful in considering fewer measurements for fault-aware control.

It was observed that features 9, 21, and 51 which correspond to reactor temperature, reactor cooling water outlet temperature, and reactor cooling water flowrate respectively were significantly more important in detecting this fault than others. These three features were used to create the described classification models.

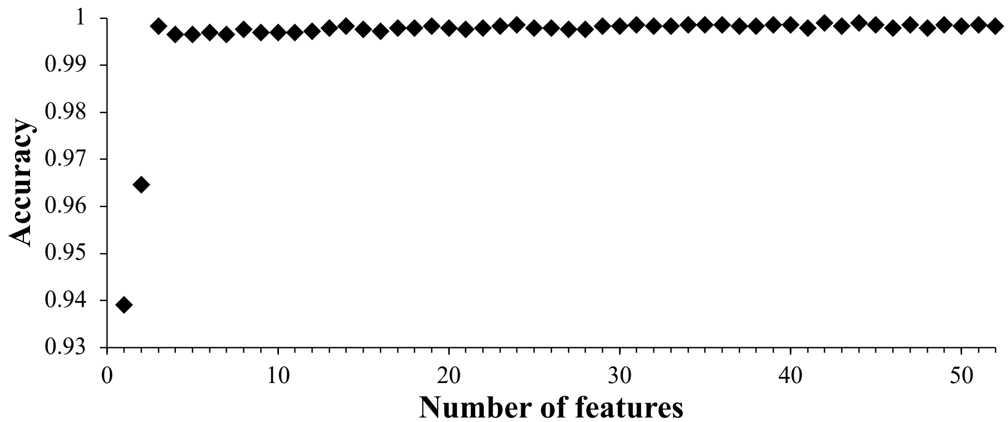


Figure 53: Average fault detection accuracy for different feature subsets

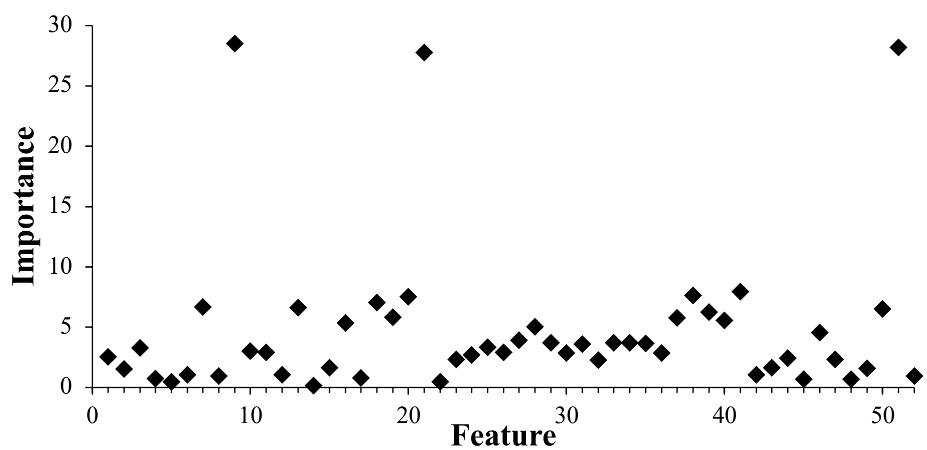


Figure 54: Average feature importance

6.4.3.3.3. Model Evaluation

A summary of the performance of the individual models and the ensemble model is shown in Table 24. It was observed that for this fault and for this data set, the models had an accuracy of over 90%. It was seen that ANN and SVM outperformed DT. It is noted that the relatively high detection performance for this fault is consistent with other work done in the literature. It is further noted that while the ensemble model performing better than the individual models could generally be expected, the absolute performance of the models would vary according to fault type and process.

Table 24: Summary of the fault detection performance of the models

Metric	ANN (%)	DT (%)	SVM (%)	Ensemble (%)
Accuracy	99.90	93.44	100.00	100.00
Sensitivity	99.88	92.25	100.00	100.00
Specificity	100.00	99.38	100.00	100.00

6.4.3.4. Explicit Control

The results presented here are for a system regime in which all three pumps are available under a pump 1 outlet cooling water valve sticking scenario. This scenario was taken to translate to a 5% decrease in pump 1 outlet flowrate from the nominal value. This effectively corresponds to the rotational speed of pump 1 being fixed at 95%. The scope of the subsequent discussion is thus for the development of a controller for pump 2, and a controller for pump 3. The output is flowrate (Q). The manipulated input is pump rotational speed (ω). The control objective is to maintain the total flowrate near 93.375 m^3/hr. It is noted that in the second case study, the controllers are made fault-aware by adjusting the flowrate setpoint of each of the other two pumps. This is shown in (147) with a fault parameter Δ of 1.55625 m^3/hr. It is further noted that the setpoints would remain unchanged in the absence of a fault.

$$y_t^{sp,new} = y_t^{sp,old} + \frac{\Delta}{2} \tag{147}$$

The mpMPC design follows the PAROC framework steps.

<u>Step 1</u>: High-fidelity dynamic modeling

A high-fidelity model of the cooling tower basin and pump network was constructed. The model equations and parameters are provided in the Supporting Information for brevity.

Step 2: Model approximation

Input-output data was generated by initializing the high-fidelity model at steady state; and then successively perturbing the rotational speed of each pump by ± 4.2% from nominal values. Surrogate model development proceeded similarly to case study 1 and resulted in a fit of 100%. It is noted that the relatively high fit performance was due to the pump affinity law between rotational speed and flowrate being linear. A plot of the surrogate model against the data, the identified state-space model, and the state-space model matrices can be found in the Supporting Information.

Step 3: Multi-parametric programming

The identified state-space model was then used to build a mpMPC controller. The parameter vector is shown in (148) and consists of a pseudo-state, and the flowrate setpoint for each pump.

$$\theta := [\theta_1, \theta_2] = \left[x_{1_{t=0}}, y_t^{sp}\right] \tag{148}$$

The control model was optimized and yielded three critical regions as shown in Figure 55.

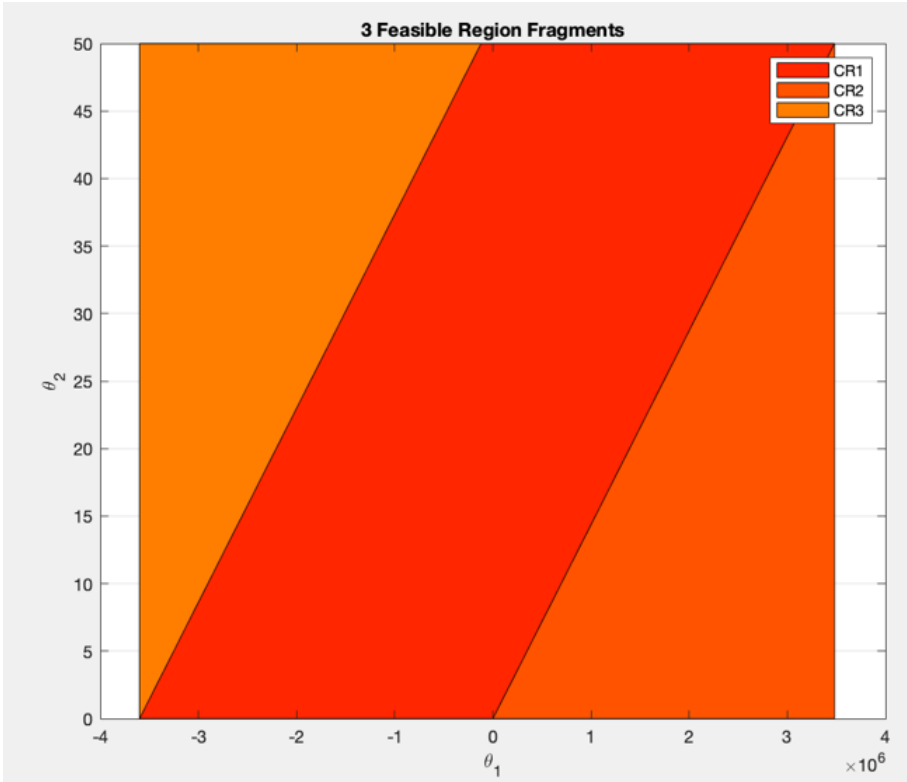


Figure 55: Case Study 2 – Control map

Step 4: Closed-loop validation

The controller was then validated against the high-fidelity model. Figure 56 shows the system in open loop and Figure 57 shows the system in closed loop. It can be seen that the fault-aware controller is able to reconfigure its control actions based on a detected process disruption.

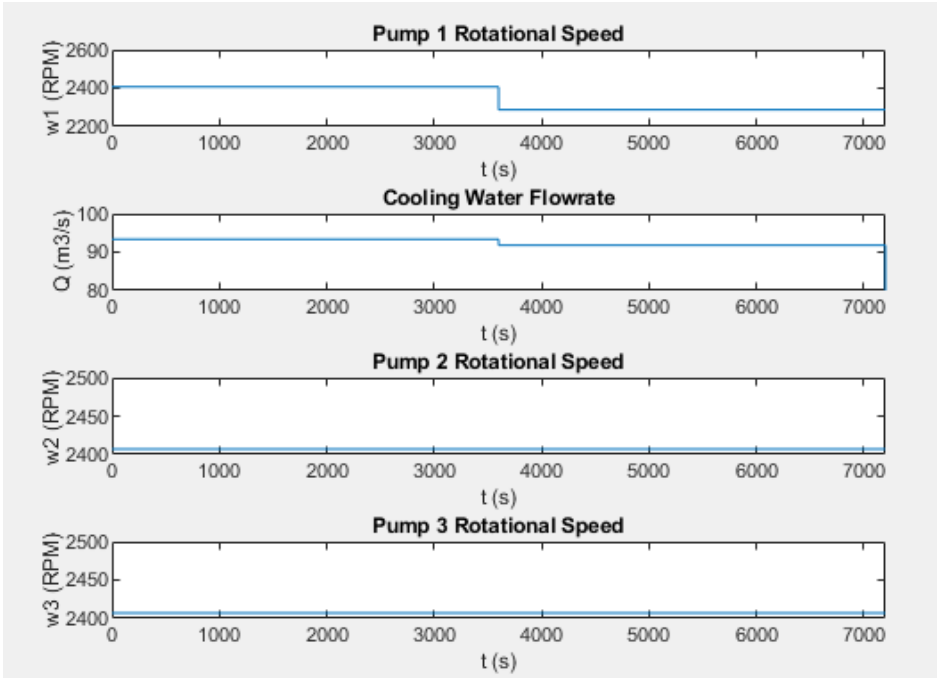


Figure 56: Case Study 2 – Non-fault aware

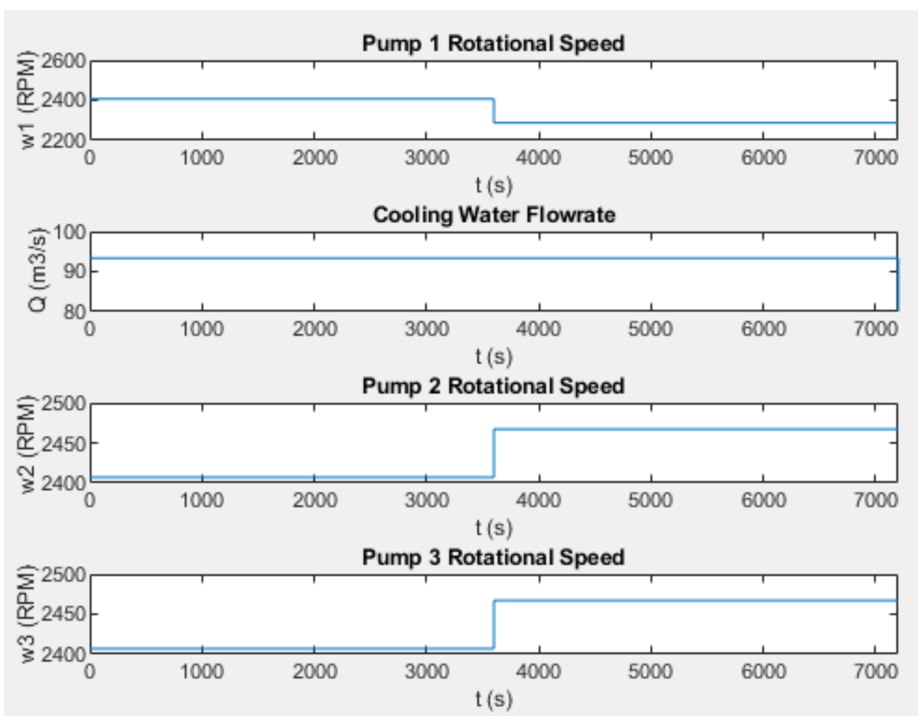


Figure 57: Case Study 2 – Closed-loop validation

6.5. Conclusions

Maintenance and production optimization can help improve the effectiveness of process systems. This paper implements a prescriptive maintenance framework for scheduling and control. The framework involves equipment failure prediction, fault detection, maintenance and production scheduling, high-fidelity dynamic simulation, and multi-parametric model predictive control. The framework was illustrated through a chemical complex case study and a cooling system case study.

Maintenance and production scheduling was done using mixed-integer nonlinear programming. Fault detection was done using an ensemble of classifiers consisting of an artificial neural network, a decision tree, and a support vector machine. It was shown that the performance of the ensemble model was equal to or better than the performance of the individual models. The scheduling and fault detection results were fed to multi-parametric model predictive controllers to obtain optimal trajectories of control actions.

Future work will be focused on extending the framework to consider simultaneous scheduling and control, startup and shutdown times, other types of faults, as well as fault diagnosis.

7. NEXT-GENERATION MAINTENANCE

7.1. Summary

This chapter provides an overview of work towards next-generation maintenance efforts and concludes with some suggestions for future work.

7.2. Biometric Data-Driven Human Reliability Analysis

7.2.1. Summary

Human and socio-organizational factors impact maintenance error probability and the overall effectiveness of production systems. However, quantifying this impact is non-trivial. Digitalization advances have led to the availability of inexpensive fitness watches and sensors that produce biometric data such as electrodermal activity data. A methodology is developed and illustrated in this section to predict maintenance error probability. This was done using a nonlinear support vector machine model to do multiclass classification on the data to predict the stress level from preprocessed electrodermal activity data. The predicted stress level was then treated as a performance shaping factor in standardized plant analysis risk human reliability analysis (SPAR-H). This yielded a stress-dependent probability of repair failure that was input into a Bayesian network to calculate the maintenance error probability. The results of the research for the system considered were a classification accuracy of 99.88% and that a high stress level increased maintenance error probability by 62.36% relative to a nominal stress level.

7.2.2. Introduction

Maintenance helps ensure process resilience and maintain system availability and avoid process safety incidents and costly losses in production. Planning and scheduling of maintenance is key, however maintenance can be erroneously executed as a result of a variety of human factors and this can influence the failure rate of plant equipment [367]. These human factors can include training, compliance, fatigue, and procedures.

Maintenance error can lead to process safety incidents. It resulted in 13% of storage tank incidents [305] and 59% of human errors in pipeline incidents [368]. In particular, maintenance error was a key factor in the 1989 Phillips 66 Pasadena, TX incident in which a valve was left open in the course of maintenance leading to the loss of containment of flammable reactor contents [369]. The resultant dispersion ignited and caused a vapor cloud explosion and severe consequences of 23 deaths, over 100 injuries, and over $500 million in economic losses [368]. As such consideration of human factors can help improve maintenance programs and system safety.

The challenge however is that human factors have a nontrivial impact on human reliability. Several human reliability analysis methods (HRAM) exist in light of this and these are summarized in Table 25. In particular, correct assignment of performance shaping factors via expert judgement is challenging. Machine learning is well positioned to assist human reliability analysis by leveraging data to improve quantification of human error probability.

Table 25: Indicative summary of related human reliability analysis literature

Reference	**Technique/Description**
[370]	Technique for human error rate prediction (THERP)
[371]	Human error assessment and reduction technique (HEART)
[372]	Cognitive reliability and error analysis method (CREAM)
[373]	A technique for human event analysis (ATHEANA)
[374]	Standardized plant analysis of risk-human reliability analysis (SPAR-H) to reflect the effect of performance shaping factors such as overall stress and fatigue on human error probability
[375]	Petro-HRA involving event trees and human error probability adjusted by performance shaping factors such as threat stress
[376]	Consider the effect of safety barriers and develop a human error probability index (HEPI)
[377]	Bayesian Networks linking mental and physiological fatigue to errors
[378]	Bayesian updating of human error probability
[379]	Ensemble support vector machine classification to predict operator performance

In this research, the performance shaping factor (PSF) of stress is determined from biometric data. This is then transformed into a human error probability of diagnostic failure using standardized plant analysis risk human reliability analysis (SPAR-H). A Bayesian network is then developed to determine maintenance effectiveness via quantification of overall maintenance error probability. The novelty of this approach is biometric data-driven human reliability analysis to help estimate maintenance error probability (MEP) via data-driven selection of PSF weights using a nonlinear support vector machine multiclass classification model. Other key features of the approach are the ability to leverage multiple data, the ability to update the Bayesian network for dynamic quantitative risk assessment, as well as the ability to tailor the predictions to individual conditions of people.

7.2.3. Problem Statement

Objectives

- Predict stress level and quantify maintenance error probability

Given

- Preprocessed electrodermal activity data
- HRAM, and PSF weights

Determine

- Stress level
- Probability of diagnostic repair error and overall MEP

7.2.4. Methodology

7.2.4.1. Machine Learning

Electrodermal activity data samples with labels corresponding to a mental state of different very high, high, nominal, or low stress levels are used to build a nonlinear support vector machine model. This model is then used for multiclass classification to determine the stress level of data samples without labels.

7.2.4.2. Human Reliability Analysis

SPAR-H is used to link performance shaping factors (PSF) $\mathrm{n} \in \mathrm{N}$ to human error probability (HEP) [374].

$$\mathrm{HEP} = \mathrm{HEP}_0 \prod_{\mathrm{n} \in \mathrm{N}} \mathrm{PSF}_{\mathrm{n}}$$

The nominal HEP is denoted HEP_0 and the performance shaping factor weights are denoted ($\mathrm{PSF}_{\mathrm{n}}$). Here stress is considered as the sole performance shaping factor and the determined stress levels from the multi-class classification are used to select the performance shaping factor weights.

7.2.4.3. Bayesian Network Analysis

A fault tree is developed for a scenario in which a maintenance action is being performed. This fault tree is then transformed into a Bayesian network (BN). The stress-dependent HEP is then used in the BN to determine the overall MEP.

7.2.5. Results

7.2.5.1. Description

The data used was preprocessed biometric electrodermal activity data [380] that was generated from the Wearable Stress and Affect Detection (WESAD) dataset [381]. The electrodermal activity data was preprocessed by signal processing, feature extraction, feature selection, and balancing, and splitting [380]. The data consists of approximately 30,000 samples of 45 biometric-related features. The outcome variable is stress level and it consists of four levels which can be described as being: ‘low’, ‘nominal, ‘high’, and ‘very high’. The data was split according to a 8:1 ratio into a training dataset and a test data set. A sample was taken randomly from the test set to use for prediction and human reliability computation. The focus of this work is purely on the model training, model evaluation, and prediction for human reliability analysis and overall maintenance error probability analysis.

7.2.5.2. Machine Learning

The support vector machine model was built on the training set with hyperparameters sigma = 0.02668296 and C = 1 using all the features. It was then evaluated on the unseen data of the test set. It had an accuracy of 99.88%, an average sensitivity of 99.49%, and an average specificity of 99.95%. The output of the machine learning step was a model. This model was used on the random sample to predict the corresponding stress level based on the feature data. The predicted stress level was ‘high’ and this was used to inform the human reliability analysis.

7.2.5.3. Human Reliability Analysis

The nominal human error probability was taken as 0.01 to reflect the default value used in SPAR-H for thinking-related diagnosis tasks [374]. The performance shaping factor values [374] for stress reflect the negative effect that it can have on tasks. It is noted that a low stress level with an arbitrarily selected weight factor has been added here to account for the positive effect of low stress on quality. It is further noted that the magnitude of this and other weight factors can be tuned.

$$\mathrm{PSF}_{\mathrm{stress}} = \begin{cases} 5, \text{Very High} \\ 2, \text{High} \\ 1, \text{Nominal} \\ 0.5, \text{Low} \end{cases}$$

The prediction from the machine learning was used to select the corresponding performance shaping factor value and calculate the human error probability.

$$\mathrm{HEP} = \mathrm{HEP}_0 \mathrm{PSF}_{\mathrm{stress}} = 0.01(2) = 0.02$$

This stress-dependent HEP was then used to determine the overall failure probability via BN.

7.2.5.4. Bayesian Network

The overall maintenance error probability analysis was done by first constructing a fault tree and then converting the fault tree into a Bayesian network. The fault tree deduces the probability of the top event of maintenance failure (M) from base events (D, E, A, T) and is shown in Figure 58.

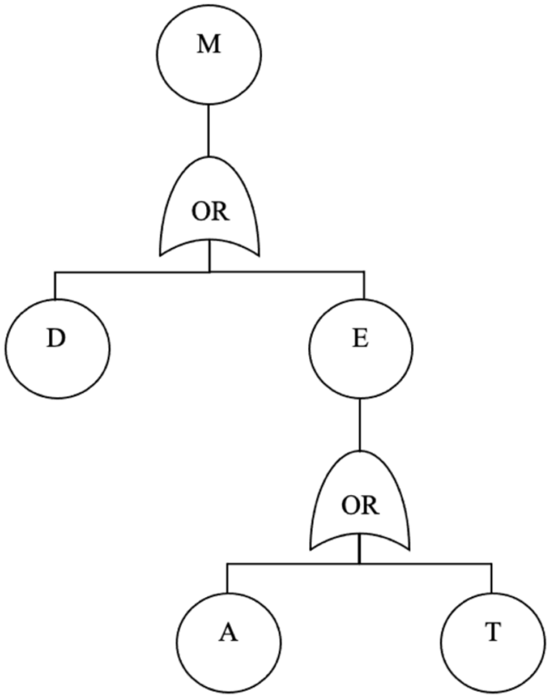


Figure 58: Maintenance error fault tree

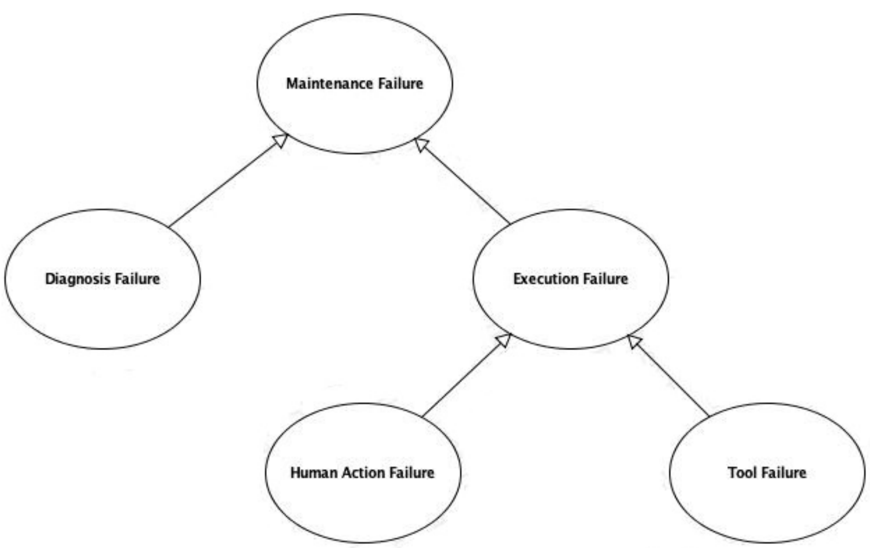


Figure 59: Maintenance error Bayesian network - Structure

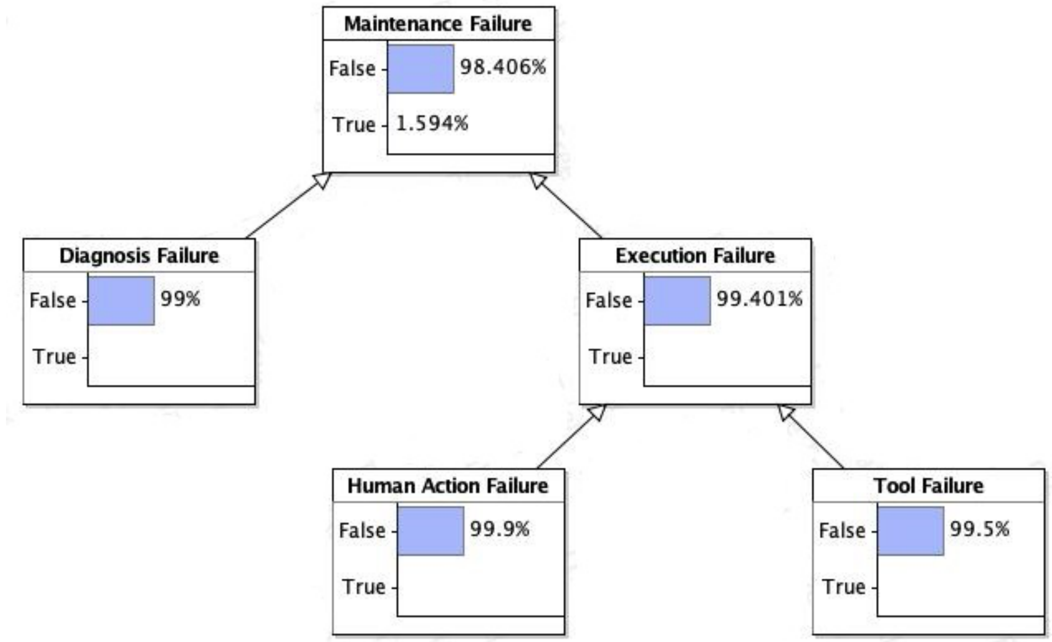


Figure 60: Maintenance error Bayesian network – Nominal stress level

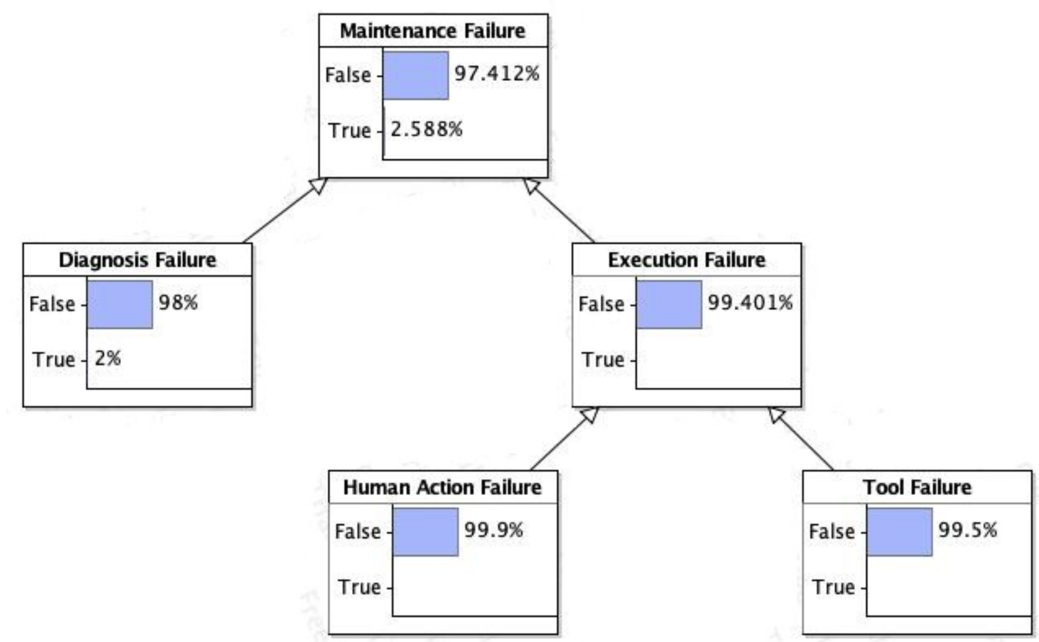


Figure 61: Maintenance error Bayesian network – High stress level

It is noted that the term maintenance failure is used here instead of maintenance error to help facilitate understanding of the fault tree and corresponding Bayesian network. It is further noted that the fault tree is highly simplified. The key base event is diagnosis failure (D) and its probability is the aforementioned stress-dependent human error probability. The other base events are human action failure (A) and tool failure (T) which contribute to task execution failure (E). The probabilities of A and T are taken as 0.001 and 0.0005 respectively.

The fault tree was converted to a Bayesian network by representing the events as Boolean variables and building in the OR gate logic into the intermediate event and top event nodes. The corresponding Bayesian network parallels the fault tree and is shown in Figure 59.

The Bayesian networks were implemented as shown in Figure 60 and Figure 61. For this example, the maintenance failure probability at a nominal stress level was 1.594% and the maintenance failure probability at a high stress level was 2.588%. It can be seen that increasing the stress level from 'nominal' to 'high' results in a 62.36% increase in maintenance failure probability.

7.2.6. Conclusions

This research developed a next-generation predictive tool for data-driven, dynamic and tailored quantitative analysis of maintenance error probability. The results of the research highlight the importance of human condition-monitoring and a human factor for maintenance effectiveness, system effectiveness, and system resilience.

7.3. Turnaround Scheduling

7.3.1. Summary

Plant turnarounds are complex endeavors that can translate to lost revenue on the order of $1 million per day. It is thus of great concern to complete all allotted tasks within the shortest time possible. This is challenging however due to uncertainty in the condition of equipment which can result in uncertain task durations, schedule overrun, and overspending. This research formulated a stochastic multi-objective optimization problem to schedule safe and cost-effective plant turnarounds while accounting for resource constraints, as well as uncertainty in task durations. This was done by solving a multi-objective discrete-time optimization model to optimality using the ε-constrained method. The model considered multiple and competing objectives of turnaround duration and resource use, considers resource constraints, and accounted for uncertainty in the mean time to repair (MTTR). The result of the research was a turnaround schedule that provided the optimal start and end times of all allotted turnaround tasks.

7.3.2. Introduction

Plant turnarounds are complex endeavors that require the completion of thousands of activities, ranging from preventive maintenance to retrofitting, by thousands of people. Plants experience partial or complete shutdowns while turnarounds are underway which can translate to lost revenue on the order of $1 million per day. As such, completing all allotted tasks within the shortest time possible is highly desirable to minimize lost revenue. Turnarounds are traditionally planned with resource management software which are driven by critical path method (CPM) algorithms which consider time, but which may not explicitly consider resource constraints. This work thus leveraged mixed-integer linear programming (MILP) to obtain optimal maintenance schedules that take resources needed into account.

7.3.3. Problem Statement

A system involving units $j \in J$, maintenance tasks $k \in K$, time intervals $t \in T$, and repair time scenarios $s \in S$.

Objectives

- Minimize turnaround duration
- Minimize resource use

Given

- Equipment mean time to repair (MTTR)
- Resource capacities

Determine

- Turnaround schedule

7.3.4. Methodology

This research uses MILP and the epsilon-constrained method.

7.3.5. Case Study

7.3.5.1. Description

The selected motivating example was a refinery with seven major production units. A single maintenance task type of generic repair was considered. A time horizon of 22 days was implemented with a time discretization of one day.

7.3.5.2. Model Formulation

Turnaround scheduling is a large resource-constrained dynamic unit task assignment problem. The model formulation involved units $j \in J = \{1,2,\dots,N_j\}$, maintenance tasks $k \in K = \{1,2,\dots,N_k\}$, time intervals $t \in T = \{0,1,2,\dots,N_t\}$, and repair time scenarios $s \in S = \{1,2,\dots,N_s\}$.

The model was a multi-stage stochastic programming model with integer recourse. The first-stage "here-and-now" decisions were the regular maintenance schedule, and the workforce capacity. The second-stage "wait-and-see" decisions were the extra recourse maintenance. Three repair time scenarios were considered consisting of the seventh production unit requiring an extra time to repair of one, two, and three days accordingly with all other unit extra repair times fixed at one day. The probability of the three scenarios were 0.2, 0.5, and 0.3 respectively.

Modeling was informed by the following considerations: (1) that unit repair time can vary, (2) that variations in repair time are accounted for by scheduling extra recourse maintenance, (3) transit and set-up time is built into the repair time distributions, and (4) that maintenance can be either regular maintenance, $m_{j,k,t} \in \{0,1\}$, or extra recourse maintenance, $e_{j,k,t,s} \in \{0,1\}$.

The objective was to minimize the expected turnaround duration or makespan (MS) which was calculated based on the last ongoing maintenance activity ($z^o_{t,s}$), a corresponding time parameter (τ_t), and probability of each scenario (p_s). Attaining this objective was subject to a set of constraints.

$$\min \mathrm{MS} \tag{149}$$

$$z^o_{t,s} \geq m_{j,k,t} + e_{j,k,t,s} \qquad \forall j \in J, \forall k \in K, \forall t \in T, \forall s \in S \tag{150}$$

$$\mathrm{MS} \geq \sum_{s=1}^{N_s} p_s \sum_{j=1}^{N_j} (\tau_t - 1)\, z^o_{t,s} \qquad \forall t \in T \tag{151}$$

No regular or recourse maintenance was permitted to occur during the first time interval, at most one type of maintenance was permitted to occur in each time interval, and at most one maintenance task type could occur on a unit at a time.

$$m_{j,k,t} = 0 \qquad \forall j \in J, \forall k \in K, \forall t = 0, \forall s \in S \tag{152}$$

$$e_{j,k,t,s} = 0 \qquad \forall j \in J, \forall k \in K, \forall t = 0, \forall s \in S \tag{153}$$

$$m_{j,k,t} + e_{j,k,t,s} \leq 1 \qquad \forall j \in J, \forall k \in K, \forall t \in T, \forall s \in S \tag{154}$$

$$\sum_{k=1}^{N_k} m_{j,k,t} \leq 1 \qquad \forall j \in J, \forall t \in T \tag{155}$$

$$\sum_{k=1}^{N_k} e_{j,k,t,s} \leq 1 \qquad \forall j \in J, \forall t \in T, \forall s \in S \tag{156}$$

The mean time to repair was split into a nominal component ($NTTR_{j,k}$), and a scenario-dependent component ($ETTR_{j,k,s}$). Regular and recourse maintenance was coerced to occur for a duration equal to the corresponding repair times.

$$\sum_{t=1}^{N_t} m_{j,k,t} = NTTR_{j,k} \qquad \forall j \in J, \forall t \in T \quad (157)$$

$$\sum_{t=1}^{N_t} e_{j,k,t,s} = ETTR_{j,k,s} \qquad \forall j \in J, \forall t \in T, \forall s \in S \quad (158)$$

Propositional logic was used to define the start and completion of maintenance activities. P_1 was used to denote maintenance at time interval t, P_2 denoted no maintenance at time interval t + 1, and P_3 denoted maintenance completion. Additionally a set of binary variables (y_1, y_2 and y_3) corresponding to the propositions was defined. It can be observed that these satisfied the following propositional logic.

$$[P_1 \wedge P_2] \rightarrow P_3 \quad (159)$$

$$\neg[P_1 \wedge P_2] \rightarrow P_3 \quad (160)$$

$$[\neg P_1 \vee \neg P_2] \vee P_3 \quad (161)$$

$$1 - y_1 + 1 - y_2 + y_3 \geq 1 \quad (162)$$

Application of the derived relationship resulted in the following set of constraints.

$$m_{j,k,t}^{start} \geq m_{j,k,t} - m_{j,k,t-1} \qquad \forall j \in J, \forall k \in K, \forall t > 1 \in T \quad (163)$$

$$m_{j,k,t}^{stop} \geq m_{j,k,t} - m_{j,k,t+1} \qquad \forall j \in J, \forall k \in K, \forall t < N_t \in T \quad (164)$$

$$e_{j,k,t,s}^{start} \geq e_{j,k,t,s} - e_{j,k,t-1,s} \qquad \forall j \in J, \forall k \in K, \forall t > 1 \in T, \forall t \in S \quad (165)$$

The obtained maintenance start and completion times enabled the following constraints which enforced contiguity of maintenance activities and linked the start of recourse maintenance to the completion of regular maintenance.

$$\sum_{t=1}^{N_t} m_{j,k,t}^{start} = 1 \qquad \forall j \in J, \forall k \in K \quad (166)$$

$$\sum_{t=1}^{N_t} m_{j,k,t}^{stop} = 1 \qquad \forall j \in J, \forall k \in K \quad (167)$$

$$\sum_{t=1}^{N_t} e_{j,k,t,s}^{start} \leq 1 \qquad \forall j \in J, \forall k \in K \quad (168)$$

$$e_{j,k,t,s}^{start} \geq m_{j,k,t-1}^{stop} \qquad \forall j \in J, \forall k \in K, \forall t > 1 \in T, \forall t \in S \quad (169)$$

The resources in terms of labor required were a function of the unit and task specific resource requirements ($l_{j,k}$). It is noted that the resources required could also be treated as being stochastic in nature, resulting in right-hand uncertainty but here the nominal value was used. The expected total resource requirements (R_t^{tot}) were then calculated and constrained to be less than total resource capacity ($R^{tot,U}$). It is noted that the constraint on the total resources used at a time corresponded to the reformulation of a the multi-objective problem involving the simultaneous minimization of makespan and resources employed at a time using the epsilon-constrained method.

$$R_{j,k,t,s} = l_{j,k}\left[m_{j,k,t} + e_{j,k,t,s}\right] \qquad \forall j \in J, \forall k \in K, \forall t \in T, \forall s \in S \quad (170)$$

$$R_t^{tot} = \sum_{s=1}^{N_s} p_s \sum_{j=1}^{N_j} \sum_{k=1}^{N_k} R_{j,k,t,s} \qquad \forall t \in T \quad (171)$$

$$R_t^{tot} \leq R^{tot,U} \qquad \forall t \in T \quad (172)$$

The formulated overall set of equations constituted a deterministic equivalent problem (DEP) and the mixed-integer linear programming model was solved using CPLEX via General Algebraic Modeling System (GAMS).

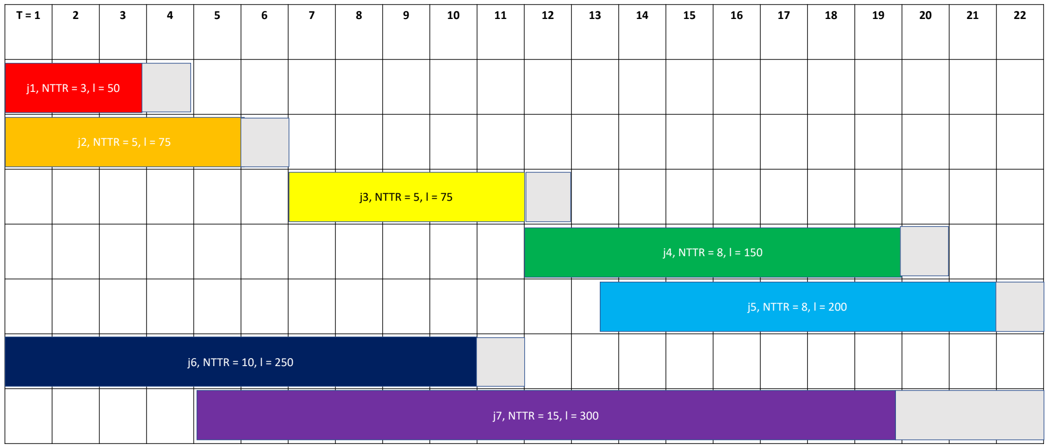


Figure 62: Turnaround schedule - Case 1

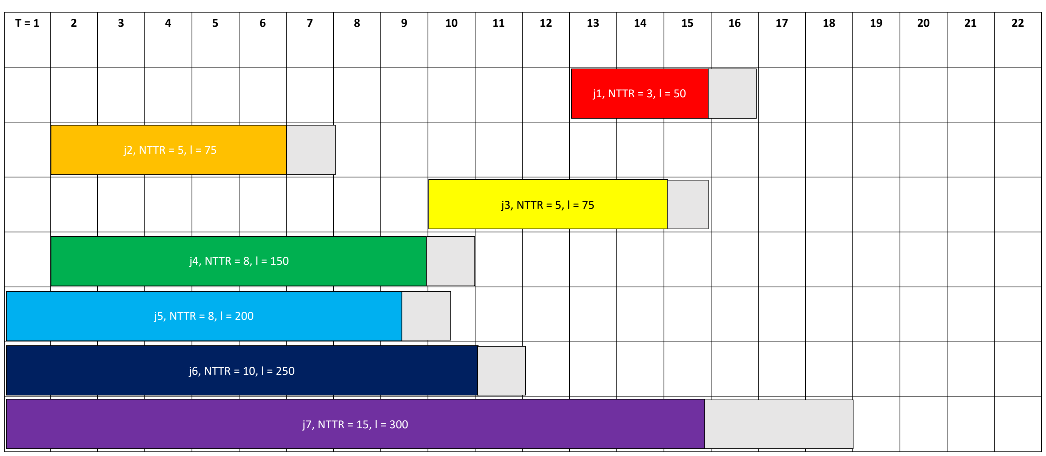


Figure 63: Turnaround schedule – Case 2

7.3.5.1. Results

Optimal turnaround schedules for the motivating example were obtained. Two cases are presented here, (1) the maximally resource constrained case shown in Figure 62, and (2) a minimally constrained case shown in Figure 63. Expected trends can be seen with Case 1 requiring more time than Case 2, and more simultaneous maintenance activities present in Case 2 than in Case 1.

It is noted that discretizing in days instead of hours resulted in an significantly smaller and more computationally tractable problem. The tradeoff however would be that scheduling smaller units requiring mean times to repair of less than a day, or scheduling non-discrete times, would result in sub-optimality.

7.3.6. Conclusions

The partial or complete shutdowns that plants experience during turnarounds can result in significant amounts of lost revenue. This is exacerbated by the presence of uncertainty in equipment condition that translates to uncertainty in the mean time to repair.

This research leveraged mixed-integer linear programming and the epsilon-constrained method for turnround scheduling. Scheduling results were obtained for a maximally resource constrained case and a minimally resource constrained case. It was seen that the turnaround activity start and end times were optimized and this research can be used to inform resource allocation and turnround decision-making.

7.4. Future Work

The data-driven approach to maintenance planning, scheduling, and control lends itself to several promising research avenues due to its predictive, simultaneous, holistic, and systematic nature. These research avenues are presently summarized.

1. Data-driven prescriptive maintenance and production planning toward environmental impact minimization: it is desirable to quantify the impact of system decisions on sustainability and develop optimal maintenance and production plans that are conscious of the environment. A sustainability-weighted expected profit metric can be developed to integrate system effectiveness with environmental impact. This would specifically involve the incorporation of a neural network into the mixed-integer nonlinear planning model to provide data-driven equipment failure probability estimates. Initial steps towards this were taken by modifying a biodiesel process [382], and simulating it in Aspen Plus as shown in Figure 64.

2. Safety-aware feature selection: the identification of the most salient measurements is typically done via the computation of an importance metric. This approach could be extended to quantify the criticality of each feature to the safety of the entire process. Specifically, this could be done by exploring the impact of the variance of each feature on a safety metric. This approach could thus involve sensitivity analysis, and or principal components analysis.

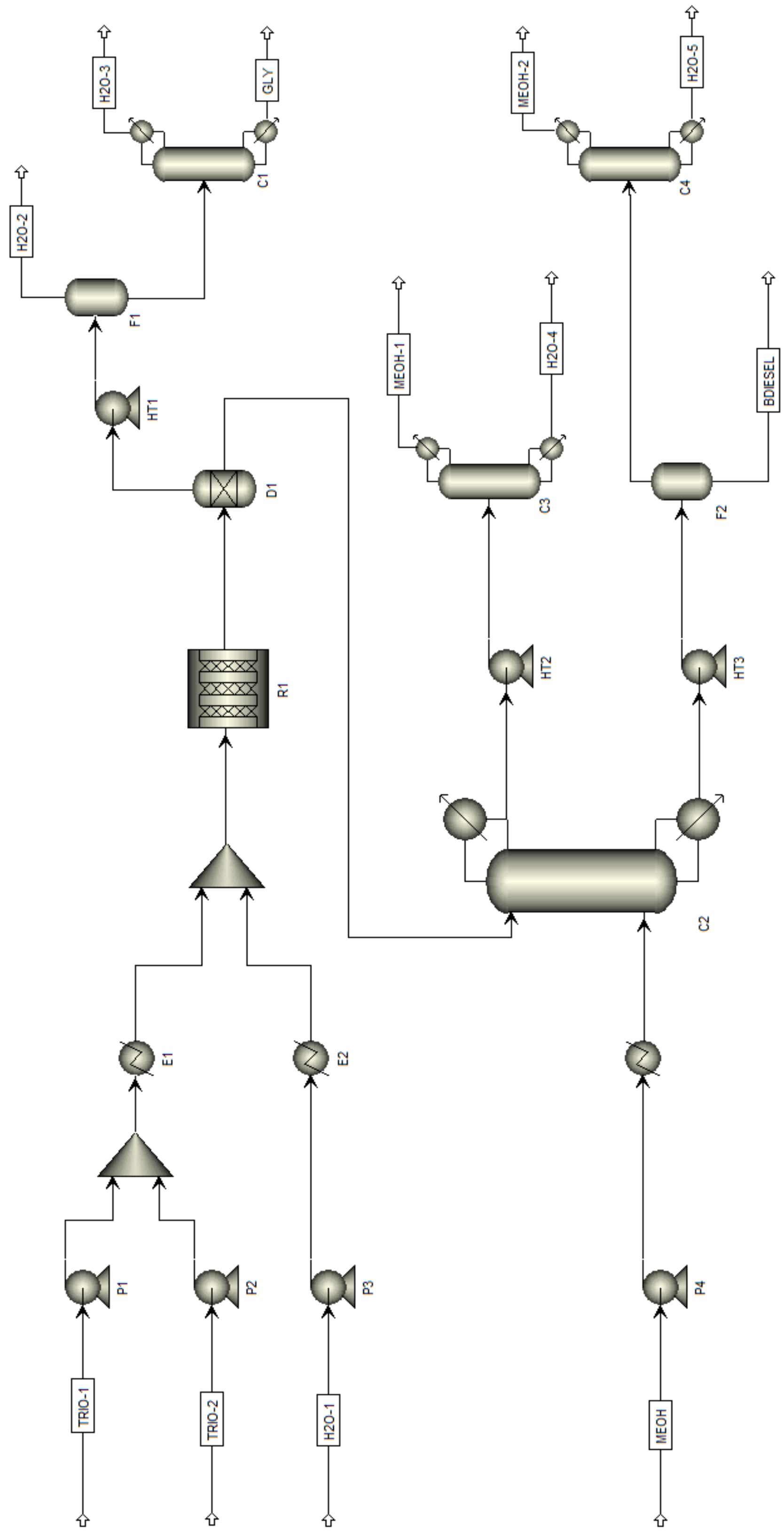


Figure 64: Biodiesel production process

3. Explicit multi-level process and maintenance optimization: it is challenging to account for uncertain parameters. These include: (1) process-related uncertainties, such as feed composition, impurities, or demand; and (2) maintenance-related uncertainties such as repair time or failure. Multiparametric optimization is well positioned to obtain optimal solutions that are a function of the uncertain parameters so as to enable rapid decision-making. However, the integrated process and maintenance optimization problem can be computationally challenging for complicated systems. As such, the process optimization problem can be considered to be a subproblem of the maintenance optimization problem and solved by adding availability to the set of process-related uncertainties. The solution to the resulting maintenance-aware multiparametric mixed integer linear programming model can be fed as affine constraints into the upper level maintenance multiparametric mixed integer linear programming model. This can be extended to add safety via trilevel optimization or constraints.

4. Hierarchical ensemble multi-class failure classification: a staggered machine learning approach can be adopted for failure prediction. Specifically, one could say develop a decision tree to first predict which quarter a failure would occur in, then predict which month of that quarter and so on. The prediction at each level could be done using ensemble classification models. The advantage of this approach is to improve predictive accuracy through tighter modeling of failure dynamics that

realize at different time scales. This approach can equally be conceptualized as coarse-graining or piecewise approximation of a nonlinear function.

5. Maintenance optimization via reinforcement learning with regret: reinforcement learning can obtain good feasible solutions to complex optimization problems. However computational time remains a challenge. As such, reinforcement learning with regret can be used to solve large mixed-integer linear programming models faster. This is done by identifying the missed benefit of alternative maintenance choices along each trajectory of decisions in each iteration and then implementing those choices on subsequent iterations to converge faster.

6. Prescriptive maintenance-aware process design: process design involves selection between alternative production routes and steady-state process flowsheet optimization. Prescriptive maintenance is complementary to this process synthesis, and allows simultaneous consideration of maintenance and disruptions to help constrain the design space and avoid sub-optimality.

7. Data-driven prescriptive maintenance toward financial risk mitigation: can help tailor the probability distributions in conditional value at risk metrics by making them both equipment condition-dependent and endogenous. This would enable better quantification of nonlinear impacts on financial losses for improved resource allocation over planning and scheduling horizons.

8. <u>'Crystal' fault propagation and safety metric</u>: from a material science perspective, the faults and failures of process monitoring and prescriptive maintenance can be considered as defects in a crystal lattice. In this way, a hybrid approach combining techniques from the field of fault propagation and materials science concepts can be developed. Specifically, the system could be modelled as being like a slice of graphite with three inter-connected and intra-connected layers: (1) a mass flow layer, (2) an energy flow layer, and (3) an information flow layer. The system is thus represented as a graph with nodes representing equipment and edges representing mass-energy-information interactions between equipment. A failure can thus be considered as a defect in the crystal lattice such as the absence of a node or edge. A fault can thus be conceptualized as a dislocation or change in the edge interaction strength. Graph theory could be used to help quantify, and elucidate complex, nonlinear, and emergent interdependencies and this could involve centrality metrics and cliques. Statistics and transfer entropy could be used to quantify the strength of dynamic, probabilistic, and nonlinear interactions to infer causality, fault propagation, and failure propagation. Furthermore, this approach could develop a safety metric by leveraging thermodynamic concepts to have a 'reference' term based on system design, and an 'excess' term based on process and maintenance decisions. This crystalline thermodynamic safety metric would change with process-maintenance interactions and could then be used for holistic planning, dynamic scheduling, and/or hybrid process control.

8. SUMMARY

This research presented a new holistic safety-aware sustainable maintenance and process optimization (SASUMAPRO) paradigm for data-driven and optimal prescriptive maintenance. It involved the development of novel methodologies to support proactive decision-making at multiple time-scales and leveraged advanced data analytics and mathematical optimization techniques. In particular it showed how machine learning could be combined with mixed-integer nonlinear programming for data-driven maintenance planning, scheduling, and control.

Planning aspects were elucidated through work on optimal multi-objective stochastic planning of preventive maintenance. This involved solving a novel multi-objective stochastic mixed-integer nonlinear optimization model to minimize cost and maximize system reliability. A set of preventive maintenance plans were obtained for use in capacity planning and inventory management.

Scheduling aspects were addressed through a novel prescriptive optimization of maintenance and process scheduling (PROMAPS) framework. This involved the development of ensembles of nonlinear support vector machine classification models for future failure prediction. Process safety was characterized through the use of a dynamic quantitative risk function that coupled consequence modeling of a vapor cloud explosion with the predicted future failure probability. The future failure prediction and risk function were then used by a multi-objective mixed-integer nonlinear programming dynamic optimization model to obtain a set of Pareto optimal solutions.

Control aspects were introduced through a novel multi-parametric-based safety-aware, maintenance-aware, and disruption-aware (mpSAMADA) framework. Failure information was used to do maintenance and production scheduling via mixed-integer nonlinear programming. Fault detection was done using an ensemble of classifiers consisting of an artificial neural network, a decision tree, and a support vector machine. It was shown that the performance of the ensemble model was equal to or better than the performance of the individual models. Multi-parametric model predictive controllers were then developed to leverage information about faults to optimal trajectories of control actions.

Next-generation maintenance research avenues were then explored. Biometric data-driven human reliability analysis via multi-class support vector machine classification was introduced for maintenance error probability prediction. Turnaround scheduling via stochastic programming and multi-objective optimization was done to minimize turnaround duration. Data-driven prescriptive maintenance and production planning towards environmental impact minimization and other ideas for future work were also presented.

This research explored the nexus of process safety engineering and process systems engineering and demonstrated steps towards the smart manufacturing industry of tomorrow. It introduced predictive approaches to proactively account for process disruptions and help reduce the likelihood of process safety incidents and their catastrophic consequences. This research contributed data-driven and optimal prescriptive maintenance approaches for simultaneous process and maintenance decision-making to help improve system resilience and system effectiveness.

9. REFERENCES

1. Okoh, P. and S. Haugen, A study of maintenance-related major accident cases in the 21st century. Process Safety and Environmental Protection, 2014. 92(4): p. 346-356.
2. Pistikopoulos, E.N., et al., Interactions of maintenance and production planning for multipurpose process plants a system effectiveness approach. Industrial & engineering chemistry research, 2001. 40(14): p. 3195-3207.
3. Nakajima, S., Introduction to TPM : total productive maintenance. 1988, Cambridge, Mass.: Productivity Press.
4. Zepf, P., OEE (Overall Equipment Effectiveness), in Wiley Encyclopedia of Packaging Technology, K. Yam, Editor. 2009, John Wiley & Sons.
5. Goel, H.D., J. Grievink, and M.P.C. Weijnen, Integrated optimal reliable design, production, and maintenance planning for multipurpose process plants. Computers & chemical engineering, 2003. 27(11): p. 1543-1555.
6. Aguirre, A.M. and L.G. Papageorgiou, Medium-term optimization-based approach for the integration of production planning, scheduling and maintenance. Computers & Chemical Engineering, 2018. 116: p. 191-211.
7. Vassiliadis, C.G. and E.N. Pistikopoulos, Maintenance scheduling and process optimization under uncertainty. Computers & Chemical Engineering, 2001. 25(2-3): p. 217-236.
8. Raouf, A., Improving capital productivity through maintenance. International Journal of Operations & Production Management, 1994.
9. Jain, P., E.N. Pistikopoulos, and M.S. Mannan, Process resilience analysis based data-driven maintenance optimization: Application to cooling tower operations. Computers & Chemical Engineering, 2019. 121: p. 27-45.
10. Crowl, D.A.L., J. F., Chemical Process Safety: Fundamentals with Applications. 2011: Pearson Education.
11. Bird, F.E., G.L. Germain, and M.D. Clark, Practical loss control leadership. 2014.
12. Hopkins, A., Thinking about process safety indicators. Safety science, 2009. 47(4): p. 460-465.
13. Safety, C.f.C.P., Recognizing Catastrophic Incident Warning Signs in the Process Industries. 2011: John Wiley & Sons, Ltd. 1-15.
14. Chakrabarty, A., S. Mannan, and T. Cagin, Multiscale modeling for process safety applications. 2015: Butterworth-Heinemann.
15. Fenton, N. and M. Neil, Rsk Assessment and Decision Analysis with Bayesian Networks. 2012: CRC Press.
16. Safety, C.f.C.P., Guidelines for Process Safety Metrics. 2009: John Wiley & Sons, Ltd.
17. Hazzan, M.J. Why is Mechanical Integrity So Tough? : American Society of Safety Engineers.
18. Ebeling, C.E., An Introduction to Reliability and Maintainability Engineering. 2010: Waveland Press.
19. Venkatasubramanian, V., The promise of artificial intelligence in chemical engineering: Is it here, finally? AIChE Journal, 2019. 65(2): p. 466-478.

20. Han, J., J. Pei, and M. Kamber, Data mining: concepts and techniques. 2011: Elsevier.
21. Kurfess, T.R., S. Billington, and S.Y. Liang, Advanced diagnostic and prognostic techniques for rolling element bearings, in Condition monitoring and control for intelligent manufacturing. 2006, Springer. p. 137-165.
22. Li, J., et al., Feature selection: A data perspective. ACM Computing Surveys (CSUR), 2017. 50(6): p. 1-45.
23. Cortes, C. and V. Vapnik, Support-vector networks. Machine learning, 1995. 20(3): p. 273-297.
24. Birge, J.R. and F. Louveaux, Introduction to stochastic programming. 2011: Springer Science & Business Media.
25. Floudas, C.A., Nonlinear and mixed-integer optimization: fundamentals and applications. 1995: Oxford University Press.
26. Haimes, Y., On a bicriterion formulation of the problems of integrated system identification and system optimization. IEEE transactions on systems, man, and cybernetics, 1971. 1(3): p. 296-297.
27. Abbasi, T., K.H. Lim, and K. San Yam. Predictive maintenance of oil and gas equipment using recurrent neural network. 2019. IOP Publishing.
28. Abu-Samah, A., et al., Failure prediction methodology for improved proactive maintenance using Bayesian approach. IFAC-PapersOnLine, 2015. 48(21): p. 844-851.
29. Amihai, I., et al. An industrial case study using vibration data and machine learning to predict asset health. 2018. IEEE.
30. Aydin, O. and S. Guldamlasioglu. Using LSTM networks to predict engine condition on large scale data processing framework. 2017. IEEE.
31. Aye, S.A. and P.S. Heyns, Prognostics of slow speed bearings using a composite integrated Gaussian process regression model. International Journal of Production Research, 2018. 56(14): p. 4860-4873.
32. Bangert, P. and S. Sharaf. Predictive maintenance for rod pumps. 2019. Society of Petroleum Engineers.
33. Baptista, M., et al., Forecasting fault events for predictive maintenance using data-driven techniques and ARMA modeling. Computers & Industrial Engineering, 2018. 115: p. 41-53.
34. Behera, S., et al. Ensemble trees learning based improved predictive maintenance using iiot for turbofan engines. 2019.
35. Bhattacharya, S. and S. Mishra, Applications of machine learning for facies and fracture prediction using Bayesian Network Theory and Random Forest: Case studies from the Appalachian basin, USA. Journal of Petroleum Science and Engineering, 2018. 170: p. 1005-1017.
36. Bhowmik, S. Life Extension of Offshore Structure Using Machine Learning. 2019. Offshore Technology Conference.
37. Bhowmik, S., Life Extension of Offshore Structure Using Machine Learning, in Offshore Technology Conference Brasil. 2019, Offshore Technology Conference: Rio de Janeiro, Brazil. p. 10.

38. Boguslawski, B., et al. Edge Analytics at the Wellhead: Designing Robust Machine Learning Models for Artificial Lift Failure Detection. 2018. Society of Petroleum Engineers.
39. Bonnevay, S., J. Cugliari, and V. Granger. Predictive maintenance from event logs using wavelet-based features: an industrial application. 2018. Springer.
40. Bruneo, D. and F. De Vita. On the use of LSTM networks for Predictive Maintenance in Smart Industries. 2019. IEEE.
41. Bukhsh, Z.A., et al., Predictive maintenance using tree-based classification techniques: A case of railway switches. Transportation Research Part C: Emerging Technologies, 2019. 101: p. 35-54.
42. Chang, G.W., Y.-H. Hong, and G.-Y. Li, A Hybrid Intelligent Approach for Classification of Incipient Faults in Transmission Network. IEEE Transactions on Power Delivery, 2019. 34(4): p. 1785-1794.
43. Chen, J., J. Chen, and X. Zhang. MTBF-oriented prediction model for airborne equipment reliability based on SOM. 2008. IEEE.
44. Cline, B., et al. Predictive maintenance applications for machine learning. 2017. IEEE.
45. Colone, L., N. Dimitrov, and D. Straub, Predictive repair scheduling of wind turbine drive-train components based on machine learning. Wind Energy, 2019. 22(9): p. 1230-1242.
46. Dindarloo, S.R. and E. Siami-Irdemoosa, Data mining in mining engineering: results of classification and clustering of shovels failures data. International Journal of Mining, Reclamation and Environment, 2017. 31(2): p. 105-118.
47. Engeler, M., et al., Condition-based maintenance: Model vs. statistics a performance comparison. Procedia CIRP, 2016. 57: p. 253-258.
48. Fong, S., et al., Automated Condition-Based Monitoring of Automated People Movers, in Automated People Movers and Automated Transit Systems 2018: Moving to the Future, Building on the Past. 2018, American Society of Civil Engineers Reston, VA. p. 57-67.
49. Gallimore, M., et al. Novelty detection for predictive maintenance scheduling for industrial gas turbines. 2011. ASME.
50. Gebraeel, N.Z., et al., Residual-life distributions from component degradation signals: A Bayesian approach. IiE Transactions, 2005. 37(6): p. 543-557.
51. Gerdes, M., Decision trees and genetic algorithms for condition monitoring forecasting of aircraft air conditioning. Expert systems with applications, 2013. 40(12): p. 5021-5026.
52. Gordon, C.A.K., et al., Data-Driven Prescriptive Maintenance: Failure Prediction Using Ensemble Support Vector Classification for Optimal Process and Maintenance Scheduling. Industrial & Engineering Chemistry Research, 2020. 59(44): p. 19607-19622.
53. Gutschi, C., et al., Log-based predictive maintenance in discrete parts manufacturing. Procedia CIRP, 2019. 79: p. 528-533.

54. Han, T., X. Liu, and A.C.C. Tan, Fault diagnosis of rolling element bearings based on Multiscale Dynamic Time Warping. Measurement, 2017. 95: p. 355-366.
55. Hanachi, H., et al. Prediction of compressor fouling rate under time varying operating conditions. 2016. American Society of Mechanical Engineers.
56. Hong, S. and Z. Zhou. Application of gaussian process regression for bearing degradation assessment. 2012. IEEE.
57. Huang, H.-P. and S.-H. Wu. Diagnostic and predictive maintenance systems for abnormal behavior of power scheduling loading and its application to robotics systems. 2011. IEEE.
58. Jin, S., et al. The Remaining Life Prediction of the Fan Bearing Based on Genetic Algorithm and Multi-Parameter Support Vector Machine. 2017. IEEE.
59. Jung, D., Z. Zhang, and M. Winslett. Vibration analysis for iot enabled predictive maintenance. 2017. IEEE.
60. Kabir, F., B. Foggo, and N. Yu. Data Driven Predictive Maintenance of Distribution Transformers. 2018. IEEE.
61. Kanawaday, A. and A. Sane. Machine learning for predictive maintenance of industrial machines using IoT sensor data. 2017. IEEE.
62. Kolokas, N., et al. Anomaly Detection in Aluminium Production with Unsupervised Machine Learning Classifiers. 2019. IEEE.
63. Koniuszewski, K. and P.D. Domański. Reproduction of equipment wear characteristics with kernel regression. 2016. IEEE.
64. Krause, J. and K. Kabitzsch. A generic Approach for Reliability Predictions considering non-uniformly Deterioration Behaviour. 2012. IOP Publishing.
65. Kumar, A., R.B. Chinnam, and F. Tseng, An HMM and polynomial regression based approach for remaining useful life and health state estimation of cutting tools. Computers & Industrial Engineering, 2019. 128: p. 1008-1014.
66. Kuzin, T. and T. Borovicka. Early Failure Detection for Predictive Maintenance of Sensor Parts. 2016.
67. Latyshev, E. Sensor Data Preprocessing, Feature Engineering and Equipment Remaining Lifetime Forecasting for Predictive Maintenance. 2018.
68. Le, T., et al. Predictive maintenance decision using statistical linear regression and kernel methods. 2014. IEEE.
69. Lee, J., et al. Smart Decision Support Tools for Robotics and Automation Systems. 2011.
70. Li, Z., et al., An ensemble learning-based prognostic approach with degradation-dependent weights for remaining useful life prediction. Reliability Engineering & System Safety, 2019. 184: p. 110-122.
71. Liu, Q., et al., Single-machine-based joint optimization of predictive maintenance planning and production scheduling. Robotics and Computer-Integrated Manufacturing, 2019. 55: p. 173-182.
72. Liu, Z.-F., et al., Improving the reliability of photovoltaic and wind power storage systems using least squares support vector machine optimized by

improved chicken swarm algorithm. Applied Sciences, 2019. 9(18): p. 3788.
73. Lygren, S., M. Piantanida, and A. Amendola. Unsupervised, Deep Learning-Based Detection of Failures in Industrial Equipments: The Future of Predictive Maintenance. 2019. Society of Petroleum Engineers.
74. Mahadevan, S. and S.L. Shah, Fault detection and diagnosis in process data using one-class support vector machines. Journal of process control, 2009. 19(10): p. 1627-1639.
75. Martinez-Rego, D., O. Fontenla-Romero, and A. Alonso-Betanzos. Power wind mill fault detection via one-class ν-SVM vibration signal analysis. 2011. IEEE.
76. Mathew, V., et al. Prediction of Remaining Useful Lifetime (RUL) of turbofan engine using machine learning. 2017. IEEE.
77. Medjaher, K., R. Gouriveau, and N. Zerhouni, A procedure for failure prognostic in dynamic systems. IFAC Proceedings Volumes, 2009. 42(4): p. 1597-1602.
78. Mitchell, W. and M. Rosner. Artificial Intelligence for Shipboard Asset Failure Prediction. 2018. The Society of Naval Architects and Marine Engineers.
79. Nixon, S., et al. A machine learning approach to diesel engine health prognostics using engine controller data. 2018.
80. Nozari, H.A., et al., Novel Non-Model-Based Fault Detection and Isolation of Satellite Reaction Wheels Based on a Mixed-Learning Fusion Framework. IFAC-PapersOnLine, 2019. 52(12): p. 194-199.
81. Onel, M., et al., Big data approach to batch process monitoring: Simultaneous fault detection and diagnosis using nonlinear support vector machine-based feature selection. Computers & chemical engineering, 2018. 115: p. 46-63.
82. Onel, M., et al., Simultaneous fault detection and identification in continuous processes via nonlinear support vector machine based feature selection, in Computer Aided Chemical Engineering. 2018, Elsevier. p. 2077-2082.
83. Pałasz, P. and R. Przysowa, Using Different ML Algorithms and Hyperparameter Optimization to Predict Heat Meters' Failures. Applied Sciences, 2019. 9(18): p. 3719.
84. Pandya, D., et al. Increasing Production Efficiency via Compressor Failure Predictive Analytics Using Machine Learning. 2018. Offshore Technology Conference.
85. Pashazadeh, V., F.R. Salmasi, and B.N. Araabi, Data driven sensor and actuator fault detection and isolation in wind turbine using classifier fusion. Renewable Energy, 2018. 116: p. 99-106.
86. Patwardhan, R.S., et al., Applications of Advanced Analytics at Saudi Aramco: A Practitioners' Perspective. Industrial & Engineering Chemistry Research, 2019. 58(26): p. 11338-11351.

87. Pinto, R. and T. Cerquitelli, Robot fault detection and remaining life estimation for predictive maintenance. Procedia Computer Science, 2019. 151: p. 709-716.
88. Proto, S., et al. PREMISES, a scalable data-driven service to predict alarms in slowly-degrading multi-cycle industrial processes. 2019. IEEE.
89. Prytz, R., et al., Predicting the need for vehicle compressor repairs using maintenance records and logged vehicle data. Engineering applications of artificial intelligence, 2015. 41: p. 139-150.
90. Raposo, H., et al., Dimensioning reserve bus fleet using life cycle cost models and condition based/predictive maintenance: a case study. Public Transport, 2018. 10(1): p. 169-190.
91. Ravi, V. and R. Patil. Unsupervised Time Series Data Analysis for Error Pattern Extraction for Predictive Maintenance. 2018. Springer.
92. Razavi, S.A., T.A. Najafabadi, and A. Mahmoodian. Remaining Useful Life Estimation Using ANFIS Algorithm: A Data-Driven Approcah for Prognostics. 2018. IEEE.
93. Rivera, D.L., et al., Towards a Predictive Maintenance System of a Hydraulic Pump. IFAC-PapersOnLine, 2018. 51(11): p. 447-452.
94. Robles-Velasco, A., et al., Prediction of pipe failures in water supply networks using logistic regression and support vector classification. Reliability Engineering & System Safety, 2020. 196: p. 106754.
95. Ruiz-Sarmiento, J.-R., et al., A predictive model for the maintenance of industrial machinery in the context of industry 4.0. Engineering Applications of Artificial Intelligence, 2020. 87: p. 103289.
96. Sadoughi, M., H. Lu, and C. Hu. A Deep Learning Approach for Failure Prognostics of Rolling Element Bearings. 2019. IEEE.
97. Salmaso, L., et al., Design of experiments and machine learning to improve robustness of predictive maintenance with application to a real case study. Communications in Statistics-Simulation and Computation, 2019: p. 1-13.
98. Scalabrini Sampaio, G., et al., Prediction of Motor Failure Time Using An Artificial Neural Network. Sensors, 2019. 19(19): p. 4342.
99. Schöpka, U., et al. Practical aspects of virtual metrology and predictive maintenance model development and optimization. 2013. IEEE.
100. Sellami, C., A. Samet, and M.A.B. Tobji. Frequent chronicle mining: Application on predictive maintenance. 2018. IEEE.
101. Shafi, U., et al., Vehicle remote health monitoring and prognostic maintenance system. Journal of advanced transportation, 2018. 2018.
102. Shin, H.J., D.-H. Eom, and S.-S. Kim, One-class support vector machines—an application in machine fault detection and classification. Computers & Industrial Engineering, 2005. 48(2): p. 395-408.
103. Shin, J.-H., Y.-S. Lee, and J.-O. Kim. Fault prediction of wind turbine by using the SVM method. 2014. IEEE.
104. Singh, K., et al. Concurrent Estimation of Remaining Useful Life for Multiple Faults in an Ion Etch Mill. 2018.

105. Smith, A.E., D.W. Coit, and Y.-C. Liang, Neural network models to anticipate failures of airport ground transportation vehicle doors. IEEE transactions on automation science and engineering, 2009. 7(1): p. 183-188.
106. Smith, H.R., E. Wiedenbrug, and M. Lind. Rotating element bearing diagnostics in a nuclear power plant: comparing vibration and torque techniques. 2007. IEEE.
107. Sotomayor, O.A.Z., et al., Observer-based supervision and fault detection of a FCC unit model predictive control system. IFAC Proceedings Volumes, 2004. 37(9): p. 523-528.
108. Sun, C., Z. Zhang, and Z. He. Research on bearing life prediction based on support vector machine and its application. 2011.
109. Susto, G.A. and A. Beghi. Dealing with time-series data in predictive maintenance problems. 2016. IEEE.
110. Susto, G.A., et al. Prediction of integral type failures in semiconductor manufacturing through classification methods. 2015. IEEE.
111. Susto, G.A., et al., A hidden-Gamma model-based filtering and prediction approach for monotonic health factors in manufacturing. Control Engineering Practice, 2018. 74: p. 84-94.
112. Susto, G.A., et al., Machine learning for predictive maintenance: A multiple classifier approach. IEEE Transactions on Industrial Informatics, 2014. 11(3): p. 812-820.
113. Turnbull, A., et al., Prediction of wind turbine generator bearing failure through analysis of high-frequency vibration data and the application of support vector machine algorithms. The Journal of Engineering, 2019. 2019(18): p. 4965-4969.
114. Verhagen, W.J.C. and L.W.M. De Boer, Predictive maintenance for aircraft components using proportional hazard models. Journal of Industrial Information Integration, 2018. 12: p. 23-30.
115. Wang, B. and Z. Mao, Outlier detection based on Gaussian process with application to industrial processes. Applied Soft Computing, 2019. 76: p. 505-516.
116. Wang, F.K. and T. Mamo, Hybrid approach for remaining useful life prediction of ball bearings. Quality and Reliability Engineering International, 2019. 35(7): p. 2494-2505.
117. Wang, J., et al., Predictive maintenance based on event-log analysis: A case study. IBM Journal of Research and Development, 2017. 61(1): p. 11-121.
118. Wiebe, J., I. Cecílio, and R. Misener, Data-driven optimization of processes with degrading equipment. Industrial & Engineering Chemistry Research, 2018. 57(50): p. 17177-17191.
119. Xayyasith, S., A. Promwungkwa, and K. Ngamsanroaj. Application of Machine Learning for Predictive Maintenance Cooling System in Nam Ngum-1 Hydropower Plant. 2018. IEEE.
120. Yang, C., et al., Machine learning-based methods for TTF estimation with application to APU prognostics. Applied Intelligence, 2017. 46(1): p. 227-239.

121. Wang, Y., et al., A cost driven predictive maintenance policy for structural airframe maintenance. Chinese Journal of Aeronautics, 2017. 30(3): p. 1242-1257.
122. You, M.-Y., et al., Statistically planned and individually improved predictive maintenance management for continuously monitored degrading systems. IEEE Transactions on Reliability, 2010. 59(4): p. 744-753.
123. Zeng, Y., et al. Prediction of equipment maintenance using optimized support vector machine. 2006. Springer.
124. Zhang, C., et al. Equipment health indicator learning using deep reinforcement learning. 2019. Springer.
125. Zhang, W., D. Yang, and H. Wang, Data-driven methods for predictive maintenance of industrial equipment: A survey. IEEE Systems Journal, 2019. 13(3): p. 2213-2227.
126. Zhang, Y., et al. Operational pattern analysis for predictive maintenance scheduling of industrial systems. 2015. IEEE.
127. Zhu, M., C. Liu, and Y. Han. An Event Correlation Based Approach to Predictive Maintenance. 2018. Springer.
128. Abedi, M., H. Seidgar, and H. Fazlollahtabar, Hybrid scheduling and maintenance problem using artificial neural network based meta-heuristics. Journal of Modelling in Management, 2017.
129. Achkar, V.G., et al., Discrete-Time MILP Formulation for the Optimal Scheduling of Maintenance Tasks on Oil and Gas Production Assets. Industrial & Engineering Chemistry Research, 2019. 58(19): p. 8231-8245.
130. Ahmed, Q., et al., A multi-constrained maintenance scheduling optimization model for a hydrocarbon processing facility. Proceedings of the Institution of Mechanical Engineers, Part O: Journal of Risk and Reliability, 2015. 229(2): p. 151-168.
131. Amaran, S., et al., Medium-term maintenance turnaround planning under uncertainty for integrated chemical sites. Computers & Chemical Engineering, 2016. 84: p. 422-433.
132. Amelian, S.S., et al., Multi-objective optimization of stochastic failure-prone manufacturing system with consideration of energy consumption and job sequences. International journal of environmental science and technology, 2019. 16(7): p. 3389-3402.
133. Antão, L., J. Reis, and G. Gonçalves. Continuous Maintenance System for optimal scheduling based on real-time machine monitoring. 2018. IEEE.
134. Arpaia, P., D. Maisto, and C. Manna. A Generalized Extremal Optimization-inspired Algorithm for Predictive Maintenance Scheduling Problems. 2010.
135. Basciftci, B., et al., Stochastic optimization of maintenance and operations schedules under unexpected failures. IEEE Transactions on Power Systems, 2018. 33(6): p. 6755-6765.
136. Bei, X., et al., Combined redundancy allocation and maintenance planning using a two-stage stochastic programming model for multiple component systems. IEEE Transactions on Reliability, 2017. 66(3): p. 950-962.

137. Bousdekis, A., et al., A proactive event-driven decision model for joint equipment predictive maintenance and spare parts inventory optimization. Procedia Cirp, 2017. 59: p. 184-189.
138. Carlos, S., A. Sánchez, and S. Martorell, Model to study the effect of workforce on a safety equipment and its optimization. Mathematical and computer modelling, 2011. 54(7-8): p. 1808-1812.
139. Carlos, S., et al., Particle Swarm Optimization of safety components and systems of nuclear power plants under uncertain maintenance planning. Advances in Engineering Software, 2012. 50: p. 12-18.
140. Castagliola, P., et al., Multiobjective optimization in an unreliable failure-prone manufacturing system. Journal of Quality in Maintenance Engineering, 2009.
141. Certa, A., et al., A multi-objective approach to optimize a periodic maintenance policy. International Journal of Reliability, Quality and Safety Engineering, 2012. 19(06): p. 1240002.
142. Chalabi, N., et al., Optimisation of preventive maintenance grouping strategy for multi-component series systems: Particle swarm based approach. Computers & Industrial Engineering, 2016. 102: p. 440-451.
143. Cheung, K.-Y., et al., Short-term site-wide maintenance scheduling. Computers & chemical engineering, 2004. 28(1-2): p. 91-102.
144. de Paula, C.P., L.B. Visnadi, and H.F. de Castro, Multi-objective optimization in redundant system considering load sharing. Reliability Engineering & System Safety, 2019. 181: p. 17-27.
145. Dedopoulos, I.T. and N. Shah, Preventive maintenance policy optimization for multipurpose plant equipment. Computers & chemical engineering, 1995. 19: p. 693-698.
146. Dedopoulos, I.T. and N. Shah, Long-term maintenance policy optimization in multipurpose process plants. Chemical engineering research & design, 1996. 74(3): p. 307-320.
147. Dekker, R., Applications of maintenance optimization models: a review and analysis. Reliability engineering & system safety, 1996. 51(3): p. 229-240.
148. Ding, F., Z. Tian, and A. Amayri, Condition-based maintenance of wind power generation systems considering different turbine types and lead times. International Journal of Strategic Engineering Asset Management, 2014. 2(1): p. 63-79.
149. Duffuaa, S.O. and K.S. Al-Sultan, A stochastic programming model for scheduling maintenance personnel. Applied Mathematical Modelling, 1999. 23(5): p. 385-397.
150. Fan, H., et al., Cooperative predictive maintenance of repairable systems with dependent failure modes and resource constraint. IEEE Transactions on Reliability, 2011. 60(1): p. 144-157.
151. Galante, G. and G. Passannanti, An exact algorithm for preventive maintenance planning of series–parallel systems. Reliability Engineering & System Safety, 2009. 94(10): p. 1517-1525.

152. Garcia, M.C., M.A. Sanz-Bobi, and J. Del Pico, SIMAP: Intelligent System for Predictive Maintenance: Application to the health condition monitoring of a windturbine gearbox. Computers in Industry, 2006. 57(6): p. 552-568.
153. Georgiadis, M.C., L.G. Papageorgiou, and S. Macchietto, Optimal cleaning policies in heat exchanger networks under rapid fouling. Industrial & engineering chemistry research, 2000. 39(2): p. 441-454.
154. Grall, A., et al., Continuous-time predictive-maintenance scheduling for a deteriorating system. IEEE transactions on reliability, 2002. 51(2): p. 141-150.
155. Hameed, A., et al., A decision support tool for bi-objective risk-based maintenance scheduling of an LNG gas sweetening unit. Journal of Quality in Maintenance Engineering, 2019.
156. Kančev, D., B. Gjorgiev, and M. Čepin, Optimization of test interval for ageing equipment: A multi-objective genetic algorithm approach. Journal of Loss Prevention in the Process Industries, 2011. 24(4): p. 397-404.
157. Khan, F.I. and M.M. Haddara, Risk-based maintenance (RBM): a quantitative approach for maintenance/inspection scheduling and planning. Journal of loss prevention in the process industries, 2003. 16(6): p. 561-573.
158. Khan, F.I. and M.R. Haddara, Risk-based maintenance of ethylene oxide production facilities. Journal of hazardous materials, 2004. 108(3): p. 147-159.
159. Kian, R., T. Bektaş, and D. Ouelhadj, Optimal spare parts management for vessel maintenance scheduling. Annals of operations research, 2019. 272(1-2): p. 323-353.
160. Kopanos, G.M., et al., Optimization of a network of compressors in parallel: Operational and maintenance planning–The air separation plant case. Applied Energy, 2015. 146: p. 453-470.
161. Kumar, E.V. and S.K. Chaturvedi, Prioritization of maintenance tasks on industrial equipment for reliability. International Journal of Quality & Reliability Management, 2011.
162. Kumar, U., et al., Maintenance performance metrics: a state-of-the-art review. Journal of Quality in Maintenance Engineering, 2013.
163. Ladj, A., F.B.-S. Tayeb, and C. Varnier. An integrated prognostic based hybrid genetic-immune algorithm for scheduling jobs and predictive maintenance. 2016. IEEE.
164. Ladj, A., et al., Exact and heuristic algorithms for post prognostic decision in a single multifunctional machine. International Journal of Prognostics and Health Management, 2017. 8(2).
165. Lao, L., M. Ellis, and P.D. Christofides, Smart manufacturing: Handling preventive actuator maintenance and economics using model predictive control. AIChE Journal, 2014. 60(6): p. 2179-2196.
166. Li, G. and D. Shi. Risk-based maintenance schedule of transmission line using multi-objective evolutionary algorithm. 2015. IEEE.
167. Li, H., et al. Integrated optimization research on preventive maintenance planning and production scheduling. 2010. IEEE.

168. Li, X., et al. Study on resource scheduling method of predictive maintenance for equipment based on knowledge. 2015. IEEE.
169. Lin, Y.-H., Y.-F. Li, and E. Zio, A framework for modeling and optimizing maintenance in systems considering epistemic uncertainty and degradation dependence based on PDMPs. IEEE Transactions on Industrial Informatics, 2017. 14(1): p. 210-220.
170. Linard, A. and M.L.P. Bueno. Towards adaptive scheduling of maintenance for cyber-physical systems. 2016. Springer.
171. Liu, B., et al., A dynamic prescriptive maintenance model considering system aging and degradation. IEEE Access, 2019. 7: p. 94931-94943.
172. Lusby, R., L.F. Muller, and B. Petersen, A solution approach based on Benders decomposition for the preventive maintenance scheduling problem of a stochastic large-scale energy system. Journal of Scheduling, 2013. 16(6): p. 605-628.
173. Manzini, R., et al., The scheduling of maintenance. A resource-constraints mixed integer linear programming model. Computers & Industrial Engineering, 2015. 87: p. 561-568.
174. Marseguerra, M., E. Zio, and L. Podofillini, A multiobjective genetic algorithm approach to the optimization of the technical specifications of a nuclear safety system. Reliability Engineering & System Safety, 2004. 84(1): p. 87-99.
175. Martón, I., et al., Optimization of test and maintenance of ageing components consisting of multiple items and addressing effectiveness. Reliability Engineering & System Safety, 2016. 153: p. 151-158.
176. Martorell, P., et al., Unavailability model for demand-caused failures of safety components addressing degradation by demand-induced stress, maintenance effectiveness and test efficiency. Reliability Engineering & System Safety, 2017. 168: p. 18-27.
177. Martorell, S., A. Sánchez, and S. Carlos, A tolerance interval based approach to address uncertainty for RAMS+ C optimization. Reliability Engineering & System Safety, 2007. 92(4): p. 408-422.
178. Martorell, S., A. Sanchez, and V. Serradell, Age-dependent reliability model considering effects of maintenance and working conditions. Reliability Engineering & System Safety, 1999. 64(1): p. 19-31.
179. Moghaddam, K.S. and J.S. Usher, A new multi-objective optimization model for preventive maintenance and replacement scheduling of multi-component systems. Engineering Optimization, 2011. 43(7): p. 701-719.
180. Nguyen, D. and M. Bagajewicz, Optimization of preventive maintenance in chemical process plants. Industrial & engineering chemistry research, 2010. 49(9): p. 4329-4339.
181. Nicolai, R.P. and R. Dekker, Optimal maintenance of multi-component systems: a review, in Complex system maintenance handbook. 2008, Springer. p. 263-286.
182. Nzukam, C., et al., Opportunistic maintenance scheduling with stochastic opportunities duration in a predictive maintenance strategy. IFAC-PapersOnLine, 2018. 51(11): p. 453-458.

183. Pan, E., W. Liao, and L. Xi, A joint model of production scheduling and predictive maintenance for minimizing job tardiness. The International Journal of Advanced Manufacturing Technology, 2012. 60(9-12): p. 1049-1061.
184. Pan, Z.j. and Y. Zhang, Transmission maintenance scheduling strategy considering potential fault risk balance. International Transactions on Electrical Energy Systems, 2015. 25(12): p. 3523-3537.
185. Paprocka, I., The model of maintenance planning and production scheduling for maximising robustness. International Journal of Production Research, 2019. 57(14): p. 4480-4501.
186. Peng, H. and G.-J. van Houtum, Joint optimization of condition-based maintenance and production lot-sizing. European Journal of Operational Research, 2016. 253(1): p. 94-107.
187. Pistikopoulos, E.N., et al., Flexibility, reliability and maintenance considerations in batch plant design under uncertainty. Computers & chemical engineering, 1996. 20: p. S1209-S1214.
188. Pistikopoulos, E.N., C.G. Vassiliadis, and L.G. Papageorgiou, Process design for maintainability: an optimization approach. Computers & Chemical Engineering, 2000. 24(2-7): p. 203-208.
189. Rajagopalan, S., et al., Risk analysis of turnaround reschedule planning in integrated chemical sites. Computers & Chemical Engineering, 2017. 107: p. 381-394.
190. Sachdeva, A., D. Kumar, and P. Kumar, Planning and optimizing the maintenance of paper production systems in a paper plant. Computers & Industrial Engineering, 2008. 55(4): p. 817-829.
191. Sanchez, A., et al., Addressing imperfect maintenance modelling uncertainty in unavailability and cost based optimization. Reliability Engineering & System Safety, 2009. 94(1): p. 22-32.
192. Si, G., et al., Triple-level opportunistic maintenance policy for leasehold service network of multi-location production lines. Reliability Engineering & System Safety, 2019. 190: p. 106519.
193. Suryadi, H. and L.G. Papageorgiou, Optimal maintenance planning and crew allocation for multipurpose batch plants. International journal of production research, 2004. 42(2): p. 355-377.
194. Susto, G.A., et al. An adaptive machine learning decision system for flexible predictive maintenance. 2014. IEEE.
195. Thomaidis, T.V. and S. Pistikopoulos. Criticality analysis of process systems. 2004. IEEE.
196. Topal, E. and S. Ramazan, A new MIP model for mine equipment scheduling by minimizing maintenance cost. European Journal of Operational Research, 2010. 207(2): p. 1065-1071.
197. Van Horenbeek, A. and L. Pintelon. Optimal prognostic maintenance planning for multi-component systems. 2012.
198. Van Horenbeek, A. and L. Pintelon, A Dynamic Prognostic Maintenance Policy for Multi-Component Systems. IFAC Proceedings Volumes, 2012. 45(31): p. 115-120.

199. Van Horenbeek, A. and L. Pintelon, A dynamic predictive maintenance policy for complex multi-component systems. Reliability engineering & system safety, 2013. 120: p. 39-50.
200. Varnier, C. and N. Zerhouni. Scheduling predictive maintenance in flow-shop. 2012. IEEE.
201. Vassiliadis, C.G., et al., Planning and maintenance optimization for multipurpose plants, in Computer Aided Chemical Engineering. 2000, Elsevier. p. 1105-1110.
202. Vassiliadis, C.G. and E.N. Pistikopoulos, Reliability and maintenance considerations in process design under uncertainty. Computers & chemical engineering, 1998. 22: p. S521-S528.
203. Vassiliadis, C.G. and E.N. Pistikopoulos, Process design and maintenance optimization under uncertainty. Computers & Chemical Engineering, 1999. 23: p. S555-S558.
204. Vassiliadis, C.G. and E.N. Pistikopoulos, Maintenance-based strategies for environmental risk minimization in the process industries. Journal of Hazardous Materials, 2000. 71(1-3): p. 481-501.
205. Wang, X., et al., Reinforcement learning based predictive maintenance for a machine with multiple deteriorating yield levels. 2014.
206. Wang, Y., et al., Development of a risk-based maintenance strategy using FMEA for a continuous catalytic reforming plant. Journal of Loss Prevention in the Process Industries, 2012. 25(6): p. 958-965.
207. Wu, S.-j., et al., A neural network integrated decision support system for condition-based optimal predictive maintenance policy. IEEE Transactions on Systems, Man, and Cybernetics-Part A: Systems and Humans, 2007. 37(2): p. 226-236.
208. Xenos, D.P., et al., Operational optimization of networks of compressors considering condition-based maintenance. Computers & Chemical Engineering, 2016. 84: p. 117-131.
209. Xia, T., et al., Optimal CBPM policy considering maintenance effects and environmental condition. The International Journal of Advanced Manufacturing Technology, 2011. 56(9-12): p. 1181-1193.
210. Xiang, Y., et al., Joint production and maintenance planning with machine deterioration and random yield. International Journal of Production Research, 2014. 52(6): p. 1644-1657.
211. Yang, Z.M., D. Djurdjanovic, and J. Ni, Maintenance scheduling in manufacturing systems based on predicted machine degradation. Journal of intelligent manufacturing, 2008. 19(1): p. 87-98.
212. Ye, Y., I.E. Grossmann, and J.M. Pinto, Mixed-integer nonlinear programming models for optimal design of reliable chemical plants. Computers & Chemical Engineering, 2018. 116: p. 3-16.
213. Ye, Y., et al., Markov chain MINLP model for reliability optimization of system design and maintenance, in Computer Aided Chemical Engineering. 2018, Elsevier. p. 1483-1488.

214. Ye, Y., et al., Modeling for reliability optimization of system design and maintenance based on Markov chain theory. Computers & Chemical Engineering, 2019. 124: p. 381-404.
215. Yildirim, M., X.A. Sun, and N.Z. Gebraeel, Sensor-driven condition-based generator maintenance scheduling—Part I: Maintenance problem. IEEE Transactions on Power Systems, 2016. 31(6): p. 4253-4262.
216. Yildirim, M., X.A. Sun, and N.Z. Gebraeel, Sensor-driven condition-based generator maintenance scheduling—part II: incorporating operations. IEEE Transactions on Power Systems, 2016. 31(6): p. 4263-4271.
217. You, M.-Y., A predictive maintenance system for hybrid degradation processes. International Journal of Quality & Reliability Management, 2017.
218. You, M.-Y., A generalized three-type lifetime probabilistic models-based hybrid maintenance policy with a practical switcher for time-based preventive maintenance and condition-based maintenance. Proceedings of the Institution of Mechanical Engineers, Part E: Journal of Process Mechanical Engineering, 2019. 233(6): p. 1231-1244.
219. You, M.-Y., et al., Cost-effective updated sequential predictive maintenance policy for continuously monitored degrading systems. IEEE Transactions on Automation Science and Engineering, 2009. 7(2): p. 257-265.
220. You, M.-Y. and G. Meng, A modularized framework for predictive maintenance scheduling. Proceedings of the institution of mechanical engineers, part O: journal of risk and reliability, 2012. 226(4): p. 380-391.
221. Zhang, P., et al. Monitoring-based task scheduling in large-scale SaaS cloud. 2016. Springer.
222. Zhou, X., L. Xi, and J. Lee, A dynamic opportunistic maintenance policy for continuously monitored systems. Journal of Quality in Maintenance Engineering, 2006.
223. Zhou, Y. and Y. Wang, A method for determining equipment to be maintained based on comprehensive risk assessment of power system. E&ES, 2018. 153(4): p. 042026.
224. Zhu, Z., et al. A sequential inspection and replacement policy for degradation-based systems. 2017. IEEE.
225. Zied, H., D. Sofiene, and R. Nidhal, Optimal integrated maintenance/production policy for randomly failing systems with variable failure rate. International Journal of Production Research, 2011. 49(19): p. 5695-5712.
226. Albalawi, F., H. Durand, and P.D. Christofides, Process operational safety using model predictive control based on a process Safeness Index. Computers & Chemical Engineering, 2017. 104: p. 76-88.
227. Allen, J.T. and N.H. El-Farra, Identification and accommodation of control actuator faults using multi-rate sampled measurements. IFAC-PapersOnLine, 2019. 52(1): p. 305-310.
228. Amin, A.A. and K.M. Hasan, A review of fault tolerant control systems: advancements and applications. Measurement, 2019. 143: p. 58-68.

229. Badihi, H., Y. Zhang, and H. Hong, Model-based active fault-tolerant cooperative control in an offshore wind farm. Energy Procedia, 2016. 103: p. 46-51.
230. Baldea, M. and I. Harjunkoski, Integrated production scheduling and process control: A systematic review. Computers & Chemical Engineering, 2014. 71: p. 377-390.
231. Benlahrache, M.A., et al., Fault Tolerant Control of Wind Turbine Using Robust Model Predictive Min-Max approach. IFAC-PapersOnLine, 2017. 50(1): p. 9902-9907.
232. Bernardi, E., C.A. Cappelletti, and E.J. Adam. Fault-tolerant Model Predictive Control Strategy Applied to Industrial Processes. 2019. IEEE.
233. Borrelli, F. and M. Morari. Offset free model predictive control. 2007. IEEE.
234. Budinis, S. and N.F. Thornhill, Control of centrifugal compressors via model predictive control for enhanced oil recovery applications. IFAC-papersonline, 2015. 48(6): p. 9-14.
235. Burnak, B., et al., Integrated process design, scheduling, and control using multiparametric programming. Computers & Chemical Engineering, 2019. 125: p. 164-184.
236. Burnak, B., N.A. Diangelakis, and E.N. Pistikopoulos, Towards the grand unification of process design, scheduling, and control—utopia or reality? Processes, 2019. 7(7): p. 461.
237. Burnak, B., et al., Simultaneous process scheduling and control: a multiparametric programming-based approach. Industrial & Engineering Chemistry Research, 2018. 57(11): p. 3963-3976.
238. Charitopoulos, V.M., L.G. Papageorgiou, and V. Dua, Closed-loop integration of planning, scheduling and multi-parametric nonlinear control. Computers & Chemical Engineering, 2019. 122: p. 172-192.
239. Chilin, D., et al., Fault detection and isolation and fault tolerant control of a catalytic alkylation of benzene process. Chemical Engineering Science, 2012. 78: p. 155-166.
240. Chilin, D., et al., Detection, isolation and handling of actuator faults in distributed model predictive control systems. Journal of Process Control, 2010. 20(9): p. 1059-1075.
241. Diangelakis, N.A., et al., Process design and control optimization: A simultaneous approach by multi-parametric programming. AIChE Journal, 2017. 63(11): p. 4827-4846.
242. Downs, J.J. and E.F. Vogel, A plant-wide industrial process control problem. Computers & chemical engineering, 1993. 17(3): p. 245-255.
243. Dua, P., F.J. Doyle, and E.N. Pistikopoulos, Multi-objective blood glucose control for type 1 diabetes. Medical & biological engineering & computing, 2009. 47(3): p. 343-352.
244. Durand, H., On accounting for equipment-control interactions in economic model predictive control via process state constraints. Chemical Engineering Research and Design, 2019. 144: p. 63-78.

245. Escobar, R.F., et al., Sensor fault compensation via software sensors: Application in a heat pump's helical evaporator. Chemical Engineering Research and Design, 2015. 93: p. 473-482.
246. Faísca, N.P., et al., A multi-parametric programming approach for multilevel hierarchical and decentralised optimisation problems. Computational management science, 2009. 6(4): p. 377-397.
247. Georgiadis, M.C., et al., Design and optimization of advanced materials and processes for efficient hydrogen storage. Computers & Chemical Engineering, 2009. 33(5): p. 1077-1090.
248. Georgiadis, M.C. and E.N. Pistikopoulos, An integrated framework for robust and flexible process systems. Industrial & engineering chemistry research, 1999. 38(1): p. 133-143.
249. Habibi, H., I. Howard, and S. Simani, Reliability improvement of wind turbine power generation using model-based fault detection and fault tolerant control: A review. Renewable Energy, 2019. 135: p. 877-896.
250. Jiang, J. and X. Yu, Fault-tolerant control systems: A comparative study between active and passive approaches. Annual Reviews in control, 2012. 36(1): p. 60-72.
251. Katz, J., B. Burnak, and E.N. Pistikopoulos, The impact of model approximation in multiparametric model predictive control. Chemical engineering research and design, 2018. 139: p. 211-223.
252. Katz, J., et al., Integrating deep learning models and multiparametric programming. Computers & Chemical Engineering, 2020: p. 106801.
253. Keller, R., et al., Fault-tolerant model predictive control of a direct methanol-fuel cell system with actuator faults. Control Engineering Practice, 2017. 66: p. 99-115.
254. Kettunen, M., P. Zhang, and S.-L. Jämsä-Jounela, An embedded fault detection, isolation and accommodation system in a model predictive controller for an industrial benchmark process. Computers & Chemical Engineering, 2008. 32(12): p. 2966-2985.
255. Koomsap, P., N.I. Shaikh, and V.V. Prabhu*, Integrated process control and condition-based maintenance scheduler for distributed manufacturing control systems. International Journal of Production Research, 2005. 43(8): p. 1625-1641.
256. Kopanos, G.M. and E.N. Pistikopoulos, Reactive scheduling by a multiparametric programming rolling horizon framework: a case of a network of combined heat and power units. Industrial & Engineering Chemistry Research, 2014. 53(11): p. 4366-4386.
257. Lao, L., et al., Real-time preventive sensor maintenance using robust moving horizon estimation and economic model predictive control. AIChE Journal, 2015. 61(10): p. 3374-3389.
258. López-Zapata, B., et al., Sensors and actuator fault tolerant control applied in a double pipe heat exchanger. Measurement, 2016. 93: p. 215-223.
259. Lucia, S., et al., Predictive control, embedded cyberphysical systems and systems of systems–A perspective. Annual Reviews in Control, 2016. 41: p. 193-207.

260. Lyman, P.R. and C. Georgakis, Plant-wide control of the Tennessee Eastman problem. Computers & chemical engineering, 1995. 19(3): p. 321-331.
261. Majdzik, P., et al., A fault-tolerant approach to the control of a battery assembly system. Control Engineering Practice, 2016. 55: p. 139-148.
262. Mendonça, L.F., J.M.C. Sousa, and J.M.G.S. da Costa, Fault tolerant control using a fuzzy predictive approach. Expert Systems with Applications, 2012. 39(12): p. 10630-10638.
263. Mohammadi, E. and M. Montazeri-Gh, Active fault tolerant control with self-enrichment capability for gas turbine engines. Aerospace Science and Technology, 2016. 56: p. 70-89.
264. Naşcu, I. and E.N. Pistikopoulos, Modeling, estimation and control of the anaesthesia process. Computers & Chemical Engineering, 2017. 107: p. 318-332.
265. Ohran, B.J., et al., Data-based fault detection and isolation using feedback control: Output feedback and optimality. Chemical engineering science, 2009. 64(10): p. 2370-2383.
266. Olivier, L.E. and I.K. Craig, Model-based fault-tolerant control with robustness to unanticipated faults. IFAC-PapersOnLine, 2017. 50(1): p. 1157-1162.
267. Onel, M., B. Burnak, and E.N. Pistikopoulos, Integrated Data-Driven Process Monitoring and Explicit Fault-Tolerant Multiparametric Control. Industrial & Engineering Chemistry Research, 2019. 59(6): p. 2291-2306.
268. Papathanasiou, M.M., et al., Intelligent, model-based control towards the intensification of downstream processes. Computers & Chemical Engineering, 2017. 105: p. 173-184.
269. Patan, K. and J. Korbicz, Fault detection and accommodation by means of neural networks. application to the boiler unit. IFAC Proceedings Volumes, 2009. 42(8): p. 119-124.
270. Pistikopoulos, E.N., et al., On-line optimization via off-line parametric optimization tools. Computers & Chemical Engineering, 2002. 26(2): p. 175-185.
271. Qin, S.J. and T.A. Badgwell, A survey of industrial model predictive control technology. Control engineering practice, 2003. 11(7): p. 733-764.
272. Ricker, N.L., Model predictive control of a continuous, nonlinear, two-phase reactor. Journal of Process Control, 1993. 3(2): p. 109-123.
273. Ricker, N.L. and J. Lee, Nonlinear model predictive control of the Tennessee Eastman challenge process. Computers & Chemical Engineering, 1995. 19(9): p. 961-981.
274. Ricker, N.L. and J. Lee, Nonlinear modeling and state estimation for the Tennessee Eastman challenge process. Computers & chemical engineering, 1995. 19(9): p. 983-1005.
275. Ringwood, J.V. and S. Simani, Overview of modelling and control strategies for wind turbines and wave energy devices: Comparisons and contrasts. Annual Reviews in Control, 2015. 40: p. 27-49.

276. Salahshoor, K. and M. Kordestani, Design of an active fault tolerant control system for a simulated industrial steam turbine. Applied Mathematical Modelling, 2014. 38(5-6): p. 1753-1774.
277. Salehifar, M., et al., Simplified fault tolerant finite control set model predictive control of a five-phase inverter supplying BLDC motor in electric vehicle drive. Electric Power Systems Research, 2016. 132: p. 56-66.
278. Sánchez-Parra, M. and C. Verde, Fault Tolerant Control with PID's for a Gas Turbine. IFAC Proceedings Volumes, 2009. 42(8): p. 1067-1072.
279. Santos, L.O., N.M.C. de Oliveira, and L.T. Biegler, Reliable and efficient optimization strategies for nonlinear model predictive control, in Dynamics and Control of Chemical Reactors, Distillation Columns and Batch Processes (Dycord'95). 1995, Elsevier. p. 33-38.
280. Sarotte, C., et al., Cryogenic Liquid Rocket Engine Test Bench Fault-Tolerant Control System: Cooling System Application. IFAC-PapersOnLine, 2019. 52(12): p. 280-285.
281. Severson, K., P. Chaiwatanodom, and R.D. Braatz, Perspectives on process monitoring of industrial systems. Annual Reviews in Control, 2016. 42: p. 190-200.
282. Shao, Q.M. and A. Cinar, System identification and distributed control for multi-rate sampled systems. Journal of Process Control, 2015. 34: p. 1-12.
283. Sheikhbahaei, R., A. Alasty, and G. Vossoughi, Robust fault tolerant explicit model predictive control. Automatica, 2018. 97: p. 248-253.
284. Sheta, A., M. Braik, and H. Al-Hiary, Modeling the Tennessee Eastman chemical process reactor using bio-inspired feedforward neural network (BI-FF-NN). The International Journal of Advanced Manufacturing Technology, 2019. 103(1-4): p. 1359-1380.
285. Shi, F. and R. Patton, An active fault tolerant control approach to an offshore wind turbine model. Renewable Energy, 2015. 75: p. 788-798.
286. Shokry, A., C. Dombayci, and A. Espuña, Multiparametric metamodels for model predictive control of chemical processes, in Computer Aided Chemical Engineering. 2016, Elsevier. p. 937-942.
287. Sourander, M., et al., Fault tolerant control for a dearomatisation process. Journal of Process Control, 2009. 19(7): p. 1091-1102.
288. Sriniwas, G.R. and Y. Arkun, Control of the Tennessee Eastman process using input-output models. Journal of Process Control, 1997. 7(5): p. 387-400.
289. Viljoen, J.H., C.J. Muller, and I.K. Craig, Hybrid nonlinear model predictive control of a cooling water network. Control Engineering Practice, 2020. 97: p. 104319.
290. Wang, L., et al., An active fault-tolerant control method based on moving window hidden Markov model. Chemical Engineering Science, 2020. 227: p. 115865.
291. Wittmann-Hohlbein, M. and E.N. Pistikopoulos, Proactive scheduling of batch processes by a combined robust optimization and multiparametric programming approach. AIChE Journal, 2013. 59(11): p. 4184-4211.

292. Wu, X. and D. Gao, Fault tolerance control of SOFC systems based on nonlinear model predictive control. International Journal of Hydrogen Energy, 2017. 42(4): p. 2288-2308.
293. Yu, X. and J. Jiang, A survey of fault-tolerant controllers based on safety-related issues. Annual Reviews in Control, 2015. 39: p. 46-57.
294. Zhang, H. and B. Lennox, Integrated condition monitoring and control of fed-batch fermentation processes. Journal of Process Control, 2004. 14(1): p. 41-50.
295. Morari, M., Design of resilient processing plants—III: A general framework for the assessment of dynamic resilience. Chemical Engineering Science, 1983. 38(11): p. 1881-1891.
296. Adedigba, S.A., F. Khan, and M. Yang, Dynamic safety analysis of process systems using nonlinear and non-sequential accident model. Chemical Engineering Research and Design, 2016. 111: p. 169-183.
297. Adedigba, S.A., F. Khan, and M. Yang, Dynamic failure analysis of process systems using principal component analysis and Bayesian network. Industrial & Engineering Chemistry Research, 2017. 56(8): p. 2094-2106.
298. Azadeh, A., et al., Combinatorial optimization of resilience engineering and organizational factors in a gas refinery by a unique mathematical programming approach. Human Factors and Ergonomics in Manufacturing & Service Industries, 2017. 27(1): p. 53-65.
299. Barua, S., et al., Bayesian network based dynamic operational risk assessment. Journal of Loss Prevention in the Process Industries, 2016. 41: p. 399-410.
300. Bhandari, J., et al., Dynamic risk-based maintenance for offshore processing facility. Process Safety Progress, 2016. 35(4): p. 399-406.
301. Boudali, H. and J.B. Dugan, A discrete-time Bayesian network reliability modeling and analysis framework. Reliability Engineering & System Safety, 2005. 87(3): p. 337-349.
302. Carlos, M., et al., Deviation propagation analysis along a cumene process by using dynamic simulations. Computers & Chemical Engineering, 2018. 117: p. 331-350.
303. Castillo-Borja, F., et al., A resilience index for process safety analysis. Journal of Loss Prevention in the Process Industries, 2017. 50: p. 184-189.
304. Čepin, M. and B. Mavko, A dynamic fault tree. Reliability Engineering & System Safety, 2002. 75(1): p. 83-91.
305. Chang, J.I. and C.-C. Lin, A study of storage tank accidents. Journal of loss prevention in the process industries, 2006. 19(1): p. 51-59.
306. Chiacchio, F., et al., SHyFTA, a Stochastic Hybrid Fault Tree Automaton for the modelling and simulation of dynamic reliability problems. Expert Systems with Applications, 2016. 47: p. 42-57.
307. Garbolino, E., J.P. Chery, and F. Guarnieri, A simplified approach to risk assessment based on system dynamics: an industrial case study. Risk Analysis, 2016. 36(1): p. 16-29.
308. Harley, A. and S.A. Maxwell. The Implementation and Automation of Effective Key Performance Indicators to manage Process Safety and Asset

Integrity Risk; a ScottishPower Case Study. 2015. Society of Petroleum Engineers.
309. Jain, P., et al., Resilience-based process upset event prediction analysis for uncertainty management using Bayesian deep learning: application to a polyvinyl chloride process system. Industrial & Engineering Chemistry Research, 2018. 57(43): p. 14822-14836.
310. Jain, P., R. Mentzer, and M.S. Mannan, Resilience metrics for improved process-risk decision making: survey, analysis and application. Safety science, 2018. 108: p. 13-28.
311. Jain, P., et al., Process Resilience Analysis Framework (PRAF): A systems approach for improved risk and safety management. Journal of Loss Prevention in the Process Industries, 2018. 53: p. 61-73.
312. Kabir, S., et al., Fuzzy temporal fault tree analysis of dynamic systems. International Journal of Approximate Reasoning, 2016. 77: p. 20-37.
313. Kalantarnia, M., F. Khan, and K. Hawboldt, Dynamic risk assessment using failure assessment and Bayesian theory. Journal of Loss Prevention in the Process Industries, 2009. 22(5): p. 600-606.
314. Kanes, R., et al., Developing a framework for dynamic risk assessment using Bayesian networks and reliability data. Journal of Loss Prevention in the Process Industries, 2017. 50: p. 142-153.
315. Khakzad, N., F. Khan, and P. Amyotte, Safety analysis in process facilities: Comparison of fault tree and Bayesian network approaches. Reliability Engineering & System Safety, 2011. 96(8): p. 925-932.
316. Khakzad, N., F. Khan, and P. Amyotte, Dynamic risk analysis using bow-tie approach. Reliability Engineering & System Safety, 2012. 104: p. 36-44.
317. Khan, F.I. and P.R. Amyotte, Integrated inherent safety index (I2SI): a tool for inherent safety evaluation. Process safety progress, 2004. 23(2): p. 136-148.
318. Khan, F.I., T. Husain, and S.A. Abbasi, Safety weighted hazard index (SWeHI): a new, user-friendly tool for swift yet comprehensive hazard identification and safety evaluation in chemical process industrie. Process Safety and Environmental Protection, 2001. 79(2): p. 65-80.
319. Khan, S.A. Process Safety-A Journey Towards Excellence. 2015. Society of Petroleum Engineers.
320. Kletz, T., What went wrong? Pump problems in the process industries. World Pumps, 1998(382): p. 45-7.
321. Knegtering, B. and H. Pasman, The safety barometer: How safe is my plant today? Is instantaneously measuring safety level utopia or realizable? Journal of Loss Prevention in the Process Industries, 2013. 26(4): p. 821-829.
322. Leveson, N., A new accident model for engineering safer systems. Safety science, 2004. 42(4): p. 237-270.
323. Marono, M., J.A. Pena, and J. Santamaria, The 'PROCESO'index: a new methodology for the evaluation of operational safety in the chemical industry. Reliability Engineering & System Safety, 2006. 91(3): p. 349-361.

324. Meel, A. and W.D. Seider, Real-time risk analysis of safety systems. Computers & Chemical Engineering, 2008. 32(4-5): p. 827-840.
325. Naderpour, M., J. Lu, and G. Zhang, An abnormal situation modeling method to assist operators in safety-critical systems. Reliability Engineering & System Safety, 2015. 133: p. 33-47.
326. Norani, A.A., et al., Risk-based interventions for safer operation of a hydrogen station. Chemical Engineering Transactions, 2017. 56: p. 1387-1392.
327. Øien, K., et al. Development of early warning indicators based on resilience engineering. 2010.
328. Paltrinieri, N., et al., Dynamic procedure for atypical scenarios identification (DyPASI): a new systematic HAZID tool. Journal of Loss Prevention in the Process Industries, 2013. 26(4): p. 683-695.
329. Roy, N., et al., A review of safety indices for process design. Current opinion in chemical engineering, 2016. 14: p. 42-48.
330. Rusli, R., A.M. Shariff, and F.I. Khan, Evaluating hazard conflicts using inherently safer design concept. Safety science, 2013. 53: p. 61-72.
331. Swaminathan, S. and C. Smidts, The event sequence diagram framework for dynamic probabilistic risk assessment. Reliability Engineering & System Safety, 1999. 63(1): p. 73-90.
332. Tugnoli, A., et al., Safety assessment in plant layout design using indexing approach: Implementing inherent safety perspective: Part 2—Domino Hazard Index and case study. Journal of Hazardous Materials, 2008. 160(1): p. 110-121.
333. Villa, V., et al., Towards dynamic risk analysis: A review of the risk assessment approach and its limitations in the chemical process industry. Safety science, 2016. 89: p. 77-93.
334. Yang, M., et al., Risk assessment of rare events. Process Safety and Environmental Protection, 2015. 98: p. 102-108.
335. Yang, X., S. Haugen, and N. Paltrinieri, Clarifying the concept of operational risk assessment in the oil and gas industry. Safety science, 2018. 108: p. 259-268.
336. Yang, X. and M.S. Mannan, The development and application of dynamic operational risk assessment in oil/gas and chemical process industry. Reliability Engineering & System Safety, 2010. 95(7): p. 806-815.
337. Yazdi, M. and S. Kabir, A fuzzy Bayesian network approach for risk analysis in process industries. Process safety and environmental protection, 2017. 111: p. 507-519.
338. Yu, H., Dynamic risk assessment of complex process operations based on a novel synthesis of soft-sensing and loss function. Process Safety and Environmental Protection, 2017. 105: p. 1-11.
339. Zhang, L. and J. Hu, Safety prognostic technology in complex petroleum engineering systems: progress, challenges and emerging trends. Petroleum Science, 2013. 10(4): p. 486-493.
340. Hollnagel, E., FRAM, the functional resonance analysis method: modelling complex socio-technical systems. 2012: Ashgate Publishing, Ltd.

341. Manca, D. and S. Brambilla, Dynamic simulation of the BP Texas City refinery accident. Journal of Loss Prevention in the Process Industries, 2012. 25(6): p. 950-957.
342. Rebennack, S. and J. Kallrath, Continuous piecewise linear delta-approximations for univariate functions: computing minimal breakpoint systems. Journal of Optimization Theory and Applications, 2015. 167(2): p. 617-643.
343. Mannan, M.S., et al., The evolution of process safety: current status and future direction. Annual review of chemical and biomolecular engineering, 2016. 7: p. 135-162.
344. D., S.O.P.B.B.Z.S.K.H.K., Predictive Maintenance. 2017, Deloitte Analytics Institute: Berlin, Germany.
345. Yazdi, M., A. Nedjati, and R. Abbassi, Fuzzy dynamic risk-based maintenance investment optimization for offshore process facilities. Journal of Loss Prevention in the Process Industries, 2019. 57: p. 194-207.
346. Onel, M., C.A. Kieslich, and E.N. Pistikopoulos, A nonlinear support vector machine-based feature selection approach for fault detection and diagnosis: Application to the Tennessee Eastman process. AIChE Journal, 2019. 65(3): p. 992-1005.
347. Bernardo, F.P., E.N. Pistikopoulos, and P.M. Saraiva, Robustness criteria in process design optimization under uncertainty. Computers & Chemical Engineering, 1999. 23: p. S459-S462.
348. Platt, J., Probabilistic outputs for support vector machines and comparisons to regularized likelihood methods. Advances in large margin classifiers, 1999. 10(3): p. 61-74.
349. Misener, R. and C.A. Floudas, ANTIGONE: algorithms for continuous/integer global optimization of nonlinear equations. Journal of Global Optimization, 2014. 59(2-3): p. 503-526.
350. Uz, F.B. Predictive Maintenance Modelling Guide Data Sets. 4/16/2019]; Available from: https://gallery.azure.ai/Experiment/Predictive-Maintenance-Implementation-Guide-Data-Sets-1. 2016.
351. Schenk, M., et al., A hybrid modelling approach for separation systems involving distillation. Chemical Engineering Research and Design, 1999. 77(6): p. 519-534.
352. Pistikopoulos, E.N., et al., PAROC—An integrated framework and software platform for the optimisation and advanced model-based control of process systems. Chemical Engineering Science, 2015. 136: p. 115-138.
353. Chiang, L.H., E.L. Russell, and R.D. Braatz, Fault diagnosis in chemical processes using Fisher discriminant analysis, discriminant partial least squares, and principal component analysis. Chemometrics and intelligent laboratory systems, 2000. 50(2): p. 243-252.
354. Cerrada, M., et al., Fault diagnosis in spur gears based on genetic algorithm and random forest. Mechanical Systems and Signal Processing, 2016. 70: p. 87-103.
355. Bemporad, A. and M. Morari, Control of systems integrating logic, dynamics, and constraints. Automatica, 1999. 35(3): p. 407-427.

356. Axehill, D., et al., A parametric branch and bound approach to suboptimal explicit hybrid MPC. Automatica, 2014. 50(1): p. 240-246.
357. Pregelj, B. and S. Gerkšič, Hybrid explicit model predictive control of a nonlinear process approximated with a piecewise affine model. Journal of Process Control, 2010. 20(7): p. 832-839.
358. Naşcu, I., R. Oberdieck, and E.N. Pistikopoulos, Explicit hybrid model predictive control strategies for intravenous anaesthesia. Computers & Chemical Engineering, 2017. 106: p. 814-825.
359. Sakizlis, V., et al. The explicit control law for hybrid systems via parametric programming. in Proceedings of the 2002 American Control Conference (IEEE Cat. No.CH37301). 2002.
360. Rivotti, P. and E.N. Pistikopoulos, A dynamic programming based approach for explicit model predictive control of hybrid systems. Computers & Chemical Engineering, 2015. 72: p. 126-144.
361. Oberdieck, R. and E.N. Pistikopoulos, Explicit hybrid model-predictive control: The exact solution. Automatica, 2015. 58: p. 152-159.
362. Avraamidou, S. and E.N. Pistikopoulos, A Multi-Parametric optimization approach for bilevel mixed-integer linear and quadratic programming problems. Computers & Chemical Engineering, 2019. 125: p. 98-113.
363. Dietterich, T.G. Ensemble methods in machine learning. Springer.
364. Tawarmalani, M. and N.V. Sahinidis, A polyhedral branch-and-cut approach to global optimization. Mathematical Programming, 2005. 103(2): p. 225-249.
365. Oberdieck, R., et al., Pop–parametric optimization toolbox. Industrial & Engineering Chemistry Research, 2016. 55(33): p. 8979-8991.
366. Serna-Gonzalez, M., J.M. Ponce-Ortega, and A. Jiménez-Gutiérrez, MINLP optimization of mechanical draft counter flow wet-cooling towers. Chemical Engineering Research and Design, 2010. 88(5-6): p. 614-625.
367. 9 - Hazard Assessment, in Lees' Loss Prevention in the Process Industries (Third Edition), S. Mannan, Editor. 2005, Butterworth-Heinemann: Burlington. p. 9/1-9/123.
368. Mannan, S., Lees' Loss Prevention in the Process Industries. 2005: Butterworth-Heinemann.
369. Sanders, R.E., 7 - Maintenance-induced accidents and process piping problems, in Chemical Process Safety (Fourth Edition), R.E. Sanders, Editor. 2015, Butterworth-Heinemann. p. 165-207.
370. Swain, A.D., Method for performing a human-factors reliability analysis. 1963, Sandia Labs., Albuquerque, N. Mex.(USA).
371. Williams, J.C. A data-based method for assessing and reducing human error to improve operational performance. 1988. IEEE.
372. Hollnagel, E., Cognitive reliability and error analysis method (CREAM). 1998: Elsevier.
373. Barriere, M., et al., Technical basis and implementation guidelines for a technique for human event analysis (ATHEANA). NUREG-1624, Rev, 2000. 1: p. 2000.

374. Gertman, D., et al., The SPAR-H human reliability analysis method. US Nuclear Regulatory Commission, 2005. 230: p. 35.
375. Bye, A., et al. Petro-HRA, a new method for human reliability analysis in the petroleum industry. 2016.
376. Deacon, T., P.R. Amyotte, and F.I. Khan, Human error risk analysis in offshore emergencies. Safety science, 2010. 48(6): p. 803-818.
377. Chen, Z., G. Qiao, and J. Zeng, Study on the relationship between worker states and unsafe behaviours in coal mine accidents based on a Bayesian Networks Model. Sustainability, 2019. 11(18): p. 5021.
378. Musharraf, M., et al., Using simulator data to facilitate human reliability analysis. Journal of Offshore Mechanics and Arctic Engineering, 2019. 141(2).
379. Zhang, X., et al., Multi-source information fusion to assess control room operator performance. Reliability Engineering & System Safety, 2020. 194: p. 106287.
380. Nkurikiyeyezu, K., A. Yokokubo, and G. Lopez, The Effect of Person-Specific Biometrics in Improving Generic Stress Predictive Models. arXiv preprint arXiv:1910.01770, 2019.
381. Schmidt, P., et al. Introducing wesad, a multimodal dataset for wearable stress and affect detection.
382. Gomez-Castro, F.I., et al., Simulation study on biodiesel production by reactive distillation with methanol at high pressure and temperature: Impact on costs and pollutant emissions. Computers & chemical engineering, 2013. 52: p. 204-215.
383. McCormick, G.P., Computability of global solutions to factorable nonconvex programs: Part I—Convex underestimating problems. Mathematical programming, 1976. 10(1): p. 147-175.
384. Al-Khayyal, F.A., Jointly constrained bilinear programs and related problems: An overview. Computers & Mathematics with Applications, 1990. 19(11): p. 53-62.
385. Meyer, C.A. and C.A. Floudas, Trilinear monomials with mixed sign domains: Facets of the convex and concave envelopes. Journal of Global Optimization, 2004. 29(2): p. 125-155.

10. APPENDIX

10.1. Literature Review Methodology

A literature review has three main goals: (1) to learn, via establishing a good knowledge base of the subject matter; (2) to scope, via identification of best practices of researchers as well as industry professionals; and (3) to identify research gaps, by providing a framework to help position future research.

Although it is impossible to have a comprehensive review of all the papers, it is possible to construct the review in such a way that it is representative. Databases leveraged included: SCOPUS, EBSCO, Web of Science, Compendex, and ScienceDirect.

Advanced searching techniques include: (1) intersecting searches, (2) using tags or controlled terms so that articles can be found regardless of if the abstract contains terms of interest, (3) proximity searches, to return articles with terms that are within a certain number of words of each other, and (4) wildcard operators.

After an initial subset of papers is defined, it is useful to update the search by looking backward to see which papers have been cited by other papers.

It is recommended to use a reference database management software such as Endnote, Refworks, Mendeley, or Rayyan.

10.2. General System Reliability Function Derivations

10.2.1. Series and Parallel

$$R_{sys,series} = \prod_{i=1}^{N} R_i$$

$$R_{sys,parallel} = 1 - \prod_{i=1}^{N} (1 - R_i)$$

10.2.2. Series-Parallel

$$R_{sys} = R_1 R_{23} = R_1[1 - (1 - R_2)(1 - R_3)] = R_1[1 - (1 - R_3 - R_2 + R_2 R_3)]$$

$$R_{sys} = R_1[R_3 + R_2 - R_2 R_3] = R_1[R_2 + R_3 - R_2 R_3]$$

$$R_{sys} = R_1 R_2 + R_1 R_3 - R_1 R_2 R_3$$

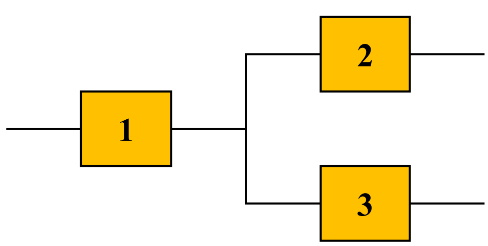


Figure S1: Series-parallel system

10.2.3. Low-Level Redundancy

$$R_{sys} = R_{12}R_{34} = [1-(1-R_1)(1-R_2)][1-(1-R_3)(1-R_4)]$$

$$R_{sys} = [R_2 + R_1 - R_1R_2)][R_4 + R_3 - R_3R_4)]$$

$$R_{sys} = [R_2R_4 + R_2R_3 - R_2R_3R_4)] + [R_1R_4 + R_1R_3 - R_1R_3R_4)] - [R_1R_2R_4 + R_1R_2R_3 - R_1R_2R_3R_4)]$$

$$R_{sys} = R_1R_3 + R_1R_4 + R_2R_3 + R_2R_4 - R_1R_3R_4 - R_2R_3R_4 - R_1R_2R_3 - R_1R_2R_4 + R_1R_2R_3R_4$$

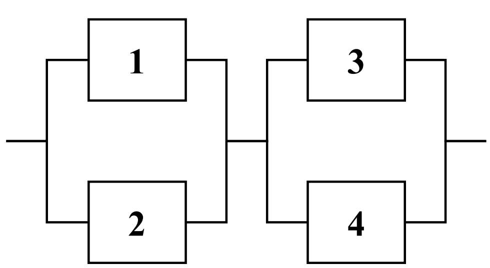


Figure S2: Low-level redundancy system

10.2.4. High-Level Redundancy

$$R_{sys} = 1 - (1 - R_{13})(1 - R_{24}) = 1 - (1 - R_1R_3)(1 - R_2R_4)$$

$$R_{sys} = 1 - (1 - R_2R_4 - R_1R_3 + R_1R_3R_2R_4)$$

$$R_{sys} = R_1R_3 + R_2R_4 - R_1R_3R_2R_4)$$

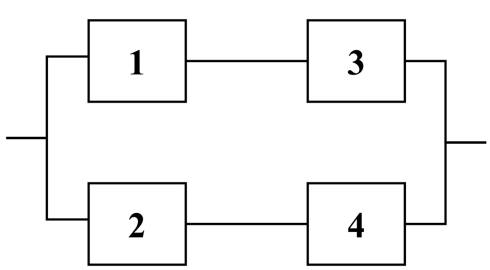


Figure S3: High-level redundancy system

10.3. Convex Envelope Derivations

10.3.1. Bilinear Convex Envelope Derivation

The bilinear term (BCC) of two continuous variables $x_1 = [x_1^L, x_1^U]$ and $x_2 = [x_2^L, x_2^U]$, is bounded from below by a convex underestimator (BCC_X) and from above by a concave overestimator (BCC_V).

The following convex underestimator was used [383]:

$$BCC_X = \max\,[x_2^U x_1 + x_1^U x_2 - x_1^U x_2^U, \qquad x_2^L x_1 + x_1^L x_2 - x_1^L x_2^L]$$

The following concave overestimator was used [384]:

$$BCC_V = \min\,[x_2^U x_1 + x_1^L x_2 - x_1^L x_2^U, \qquad x_2^L x_1 + x_1^U x_2 - x_1^U x_2^L]$$

The bilinear term is thus approximated by the following set of inequalities

$$BCC \geq x_2^U x_1 + x_1^U x_2 - x_1^U x_2^U$$

$$BCC \geq x_2^L x_1 + x_1^L x_2 - x_1^L x_2^L$$

$$BCC \leq x_2^U x_1 + x_1^L x_2 - x_1^L x_2^U$$

$$BCC \leq x_2^L x_1 + x_1^U x_2 - x_1^U x_2^L$$

10.3.2. Trilinear Convex Envelope Derivation

Given a trilinear term term (TCCC) of three continuous variables $x_1 = [x_1^L, x_1^U]$, $x_2 = [x_2^L, x_2^U]$, and $x_3 = [x_3^L, x_3^U]$ satisfying the following relations [385]:

$$x_1 \geq 0$$

$$x_2 \geq 0$$

$$x_3 \geq 0$$

$$x_1^U x_2^L x_3^L + x_1^L x_2^U x_3^U \leq x_1^L x_2^U x_3^L + x_1^U x_2^L x_3^U$$

$$x_1^U x_2^L x_3^L + x_1^L x_2^U x_3^U \leq x_1^U x_2^U x_3^L + x_1^L x_2^L x_3^U$$

Defining $\varphi_1 = x_1^U x_2^U x_3^L - x_1^L x_2^U x_3^U - x_1^U x_2^L x_3^L + x_1^U x_2^L x_3^U$, and $\varphi_2 = x_1^L x_2^L x_3^U - x_1^U x_2^L x_3^L - x_1^L x_2^U x_3^U + x_1^L x_2^U x_3^L$, the trilinear term is thus approximated by the following inequalities:

$$\mathrm{TCCC} \geq x_2^L x_3^L x_1 + x_1^L x_3^L x_2 + x_1^L x_2^L x_3 - 2x_1^L x_2^L x_3^L$$

$$\mathrm{TCCC} \geq x_2^U x_3^U x_1 + x_1^U x_3^U x_2 + x_1^U x_2^U x_3 - 2x_1^U x_2^U x_3^U$$

$$\mathrm{TCCC} \geq x_2^L x_3^U x_1 + x_1^L x_3^U x_2 + x_1^U x_2^L x_3 - x_1^L x_2^L x_3^U - x_1^U x_2^L x_3^U$$

$$\mathrm{TCCC} \geq x_2^U x_3^L x_1 + x_1^U x_3^L x_2 + x_1^L x_2^U x_3 - x_1^U x_2^U x_3^L - x_1^L x_2^U x_3^L$$

$$\mathrm{TCCC} \geq \frac{\varphi_1}{x_1^U - x_1^L} x_1 + x_1^U x_3^L x_2 + x_1^U x_2^L x_3$$

$$+ \left(-\frac{\varphi_1 x_1^L}{x_1^U - x_1^L} - x_1^U x_2^U x_3^L - x_1^U x_2^L x_3^U + x_1^L x_2^U x_3^U \right)$$

$$\mathrm{TCCC} \geq \frac{\varphi_2}{x_1^L - x_1^U} x_1 + x_1^L x_3^U x_2 + x_1^L x_2^U x_3$$

$$+ \left(-\frac{\varphi_2 x_1^U}{x_1^L - x_1^U} - x_1^L x_2^L x_3^U - x_1^L x_2^U x_3^L + x_1^U x_2^L x_3^L \right)$$

$$\mathrm{TCCC} \leq x_2^L x_3^L x_1 + x_1^U x_3^L x_2 + x_1^U x_2^U x_3 - x_1^U x_2^U x_3^L - x_1^U x_2^L x_3^L$$

$$\mathrm{TCCC} \leq x_2^U x_3^L x_1 + x_1^L x_3^L x_2 + x_1^U x_2^U x_3 - x_1^U x_2^U x_3^L - x_1^L x_2^U x_3^L$$

$$\mathrm{TCCC} \leq x_2^L x_3^L x_1 + x_1^U x_3^U x_2 + x_1^U x_2^L x_3 - x_1^U x_2^L x_3^U - x_1^U x_2^L x_3^L$$

$$\mathrm{TCCC} \leq x_2^U x_3^U x_1 + x_1^L x_3^L x_2 + x_1^L x_2^U x_3 - x_1^L x_2^U x_3^U - x_1^L x_2^U x_3^L$$

$$\mathrm{TCCC} \leq x_2^L x_3^U x_1 + x_1^U x_3^U x_2 + x_1^L x_2^L x_3 - x_1^U x_2^L x_3^U - x_1^L x_2^L x_3^U$$

$$\mathrm{TCCC} \leq x_2^U x_3^U x_1 + x_1^L x_3^U x_2 + x_1^L x_2^L x_3 - x_1^L x_2^U x_3^U - x_1^L x_2^L x_3^U$$

10.3.3. Simplified Bilinear and Trilinear Convex Envelope Derivation

The aforementioned bilinear and trilinear convex envelopes can be simplified.

For $x_1 = [x_1^L, x_1^U] = [0,1]$ and $x_2 = [x_2^L, x_2^U] = [0,1]$, the convex envelope of a bilinear term can be represented by the following set of linear inequalities:

$\mathrm{BCC} \geq x_1 + x_2 - 1$

$\mathrm{BCC} \geq 0$

$\mathrm{BCC} \leq x_1$

$\mathrm{BCC} \leq x_2$

For $x_1 = [x_1^L, x_1^U] = [0,1]$, $x_2 = [x_2^L, x_2^U] = [0,1]$, and $x_3 = [x_3^L, x_3^U] = [0,1]$ and with redundant inequalities removed, the convex envelope of a trilinear term can be represented by the following set of linear inequalities:

$\mathrm{TCCC} \geq 0$

$\mathrm{TCCC} \geq x_1 + x_2 + x_3 - 2$

$\mathrm{TCCC} \leq x_3$

$\mathrm{TCCC} \leq x_2$

$\mathrm{TCCC} \leq x_1$

10.4. Supporting Information for Chapter 5

10.4.1. Event Tree Analysis

It is desired to prevent, mitigate, and respond (PMR) to process safety incidents. In the event of failure of prevention measures leading to a loss of containment (LOC) and release of process fluid, various event sequences can occur and can be analyzed using an event tree. Scenario analysis was first done considering leak as the initiating event. The pump subsystem has a series of mitigation measures which serve as event propagation barriers, and they consist of an automatic and remotely operated emergency shut-off valve (ESV) that relies on the activation of a gas detection system.

Qualitative event tree analysis provides a succinct representation of the possible event sequences and can be used for communication as well as to enable quantitative analysis. The immediate event following the loss of containment of process fluid would be the formation of a pool of flammable liquid which lead to a pool fire if a nearby ignition source is found. Given that some of the released process fluid would flash immediately at ambient conditions, and that some of the liquid pool would vaporize, there would be the formation of a vapor cloud. The ESV serves to limit the amount of process fluid lost and if activated, leads to the formation of a smaller vapor cloud and a larger vapor cloud otherwise. Depending on atmospheric conditions, the vapor cloud can be eventually dispersed, however if an ignition source is found, there can be delayed ignition of the vapor cloud and a vapor cloud explosion (VCE).

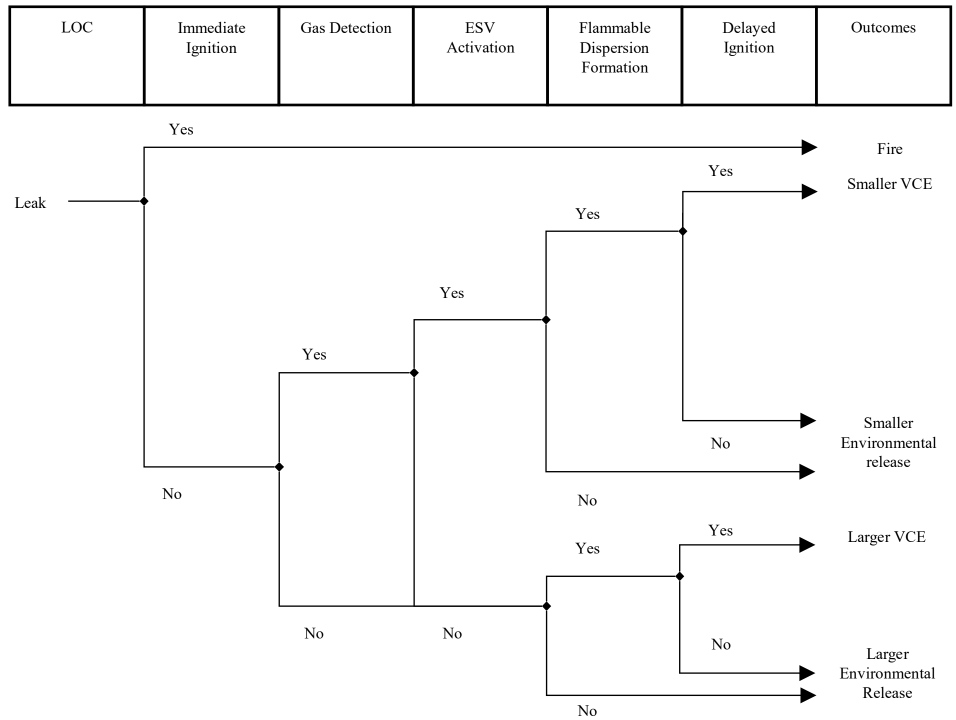


Figure S4: Hydrocarbon system event tree

The event tree analysis identified outcome events of environmental release, fire, vapor cloud explosion (VCE). The intermediate event probabilities for ignition, gas detection, ESV activation, flammable dispersion formation and delayed ignition were taken to be 0.05, 0.95, 0.99, 1, and 0.1 respectively. Quantitative event tree analysis resulted in outcome event probabilities for environmental release, VCE, and fire being 0.847, 0.094, and 0.050 respectively. It was assumed that the environmental release without ignition would disperse to the atmosphere. VCE was thus selected for further analysis.

10.4.2. Parameters

Table S1: Case Study 1 – Parameters

Parameter	Symbol	Value
Heat transfer area, m^2	A	13.5
Process stream inlet concentration, $kmol/m^3$	C_{A0}	32.04
Mixture heat capacity, kJ/(kmol K)	C_p	167.4
Water heat capacity, kJ/(kg K)	C_p^w	4.18
Minimum flowrate, kmol/hr	F^L	10
Maximum flowrate, kmol/hr	F^U	100000
Minimum water flowrate, kg/hr	$F^{w,L}$	227.1
Maximum water flowrate, kg/hr	$F^{w,U}$	5000
Maximum temperature, K	$\mathbb{T}^{max}$	389
Safety margins, K	$\mathbb{T}^{\Delta}$	[20 , 30, 35, 40, 50]
Ratio of activation energy to gas constant, K	E/R	555.6
Arrhenius rate factor, hr^{-1}	k	0.6242
Mean time to repair, hr	MTTR	4
Sampling horizon	N_s	12
Ensemble size	N_G	12
Heat of reaction, kJ/kmol	ΔH_{rxn}	23260
Minimum process temperature	$\mathbb{T}^L$	311
Temperature threshold, K	$\mathbb{T}^U$	389
Process stream inlet temperature, K	$\mathbb{T}_0$	333.3
Water inlet temperature, K	$\mathbb{T}_{w1}$	300
Minimum water outlet temperature, K	$\mathbb{T}_{w1}^L$	301
Maximum water outlet temperature, K	$\mathbb{T}_{w2}^U$	356
Heat transfer coefficient, kJ/(m^2 hr K)	U	1635.34
Reactor volume, m^3	V	40

Table S2: Case Study 2 – Parameters

Parameter	Symbol	Value
Process		
Feed composition	$FEED\_X_I$	[0.09, 0.3, 0.5, 0.1, 0.01]
Feed nominal flowrates, kmol/hr	F_i^n	[324, 1080, 1800, 360, 36]
Feed flow bounds, kmol/hr	$FEED^L, FEED^U$	[3240, 3960]
Feed temperature, °C	T_{s1}	25
Flow bounds, kmol/hr	F^L, F^U	[0,6300]
Reflux ratio bounds	R^L, R^U	[2.25, 2.75]
Pump efficiency	η_j	[0.7, 0.65]
Density, kg/m^3	ρ	484
Acceleration due to gravity, m/s^2	g	9.81
Average head, m	H	124
Conversion constant	χ	3.6×10^6
Lower production targets, kmol/hr	$PROD\_TARGET_t^L$	[1000, 1025, 1050, 1025, 1025, 1050, 1050]
Upper production targets, kmol/hr	$PROD\_TARGET_t^U$	[1075, 1100, 1125, 1100, 1100, 1125, 1125]
Safety		
Conditional probability of seal failure, yr^{-1}	P_f	0.00068
Probability of standby pump failure	$P_{P2}^{m,f}$	0.001
Explosion efficiency	η_{ex}	0.02
Release duration, hr	t^r	0.016667
TNT explosion energy, kJ	E^{TNT}	4686
Heat of combustion, kJ/mol	C_{p_B}	2219.2
Overpressure distance, m	r^{TNT}	20
Scaled distance bounds, m/kg$^{1/3}$	$z^{TNT,L}, z^{TNT,U}$	[0,35]
Equivalent mass of TNT bounds, kg	$m^{TNT,L}, m^{TNT,U}$	[0,25000]
Thresholds (10^{-4})	$\bar{\Lambda}_l$	[1.696, 1.694, 1.693, 1.691, 1.690 1.689, 1.687, 1.686, 1.685, 1.683]

Table S2: Continued

Parameter	Symbol	Value
Maintenance		
Sampling horizon	$\mathrm{N_s}$	12
Ensemble size	$\mathrm{N_G}$	12
Mean time to repair, hr	MTTR	4
Periods before pump changeover	κ	8
Weibull scale parameter	α	2
Weibull shape parameter	β	1.25
Economic		
Value of species, $/kmol	$\mathrm{V_i}$	[3.05, 8.79, 14.97, 30.09, 0]
Labor cost, $/hr	$\mathrm{C^l}$	16
Maintenance cost, $/hr	$\mathrm{C^m}$	200
Coldwater cost, $/kJ	$\mathrm{C^{u1}}$	2×10^{-7}
MP steam cost, $/kJ	$\mathrm{C^{u2}}$	2.5×10^{-6}
Electricity cost, $/kWh	$\mathrm{C^e}$	0.12
Resources		
Power capacity, kWh	ERC	10000
Human resource capacity	HRC	3
Human resources required	HRR	1
Maintenance resource capacity	MRC	2
Maintenance resources required	MRR	1

* Each specified production targets is for 24 hours

10.4.3. Phase 1 - Preprocessing

Table S3: Head of raw pooled data

Time	Voltage	Rotation	Vibration	Next time of failure	Last time of maintenance	Errors to date
1/1/15 6:00	176.22	418.50	45.09	1/5/15 6:00	7/16/14 6:00	0
1/1/15 7:00	162.88	402.75	43.41	1/5/15 6:00	7/16/14 6:00	0
1/1/15 8:00	170.99	527.35	34.18	1/5/15 6:00	7/16/14 6:00	0
1/1/15 9:00	162.46	346.15	41.12	1/5/15 6:00	7/16/14 6:00	0
1/1/15 10:00	157.61	435.38	25.99	1/5/15 6:00	7/16/14 6:00	0

Table S4: Head of processed pooled data

volt	volt_mean	volt_min	volt_max	volt_stdev	volt_RMS
-0.6977	-0.7124	1.1310	-2.0609	-2.5436	-0.7957
-1.1492	-1.0538	0.7716	-2.1586	-2.4239	-1.1343
0.7708	-0.7573	0.7716	-1.3475	-1.9095	-0.8257
-0.0396	-0.7671	0.7716	-1.3475	-1.9184	-0.8357

Table S4: Continued

rotation	rotation_mean	rotation_min	rotation_max	rotation_stdev	rotation_RMS
0.0239	-0.8662	-0.6299	-0.0533	0.0771	-0.8743
0.8484	-0.5586	-0.6299	-0.0533	0.3475	-0.5492
-0.5547	-0.4927	-0.6299	-0.0533	0.2790	-0.4869
-0.8593	-1.0250	-0.6299	-0.9561	-0.4793	-1.0638

Table S4: Continued

vibration	vibration_mean	vibration_min	vibration_max	vibration_stdev	vibration_RMS
-0.3732	-0.5366	-1.8628	-0.8839	0.5802	-0.5074
0.6272	-0.5672	-1.8628	-0.8839	0.5013	-0.5419
0.1344	-0.6313	-1.8628	-0.8839	0.3975	-0.6107
-0.1582	-0.4573	-1.8628	-0.8839	0.2066	-0.4483

Table S4: Continued

TSLM	TSLM_mean	TSLM_min	TSLM_max	TSLM_stdev	TSLM_RMS
0.7854	0.7849	0.7927	0.7731	-0.0873	0.7823
0.7858	0.7853	0.7932	0.7735	-0.0873	0.7827
0.7862	0.7857	0.7936	0.7739	-0.0873	0.7831
0.7867	0.7862	0.7940	0.7744	-0.0873	0.7835

Table S4: Continued

ESLM	ESLM_mean	ESLM_min	ESLM_max	ESLM_stdev	ESLM_RMS
-0.9852	-0.9889	-0.9783	-0.9949	-0.1404	-0.9913
-0.9852	-0.9889	-0.9783	-0.9949	-0.1404	-0.9913
-0.9852	-0.9889	-0.9783	-0.9949	-0.1404	-0.9913
-0.9852	-0.9889	-0.9783	-0.9949	-0.1404	-0.9913

Table S4: Continued

Y1…Y80	Y_81	Y_82	Y_83	Y_84	Y_85	Y86…Y168
0	0	0	0	0	1	1
0	0	0	0	1	1	1
0	0	0	1	1	1	1
0	0	1	1	1	1	1

It is noted that that here, $N_k = 168$, and that the processed pooled data set is split into 168 data sets by pairing the input features with each extracted outcome (Y_k). Feature selection and model creation proceed by considering each data set k in turn.

10.4.4. Phase 2 – Feature Selection

10.4.4.1. Overview

It can be observed above that there are 30 input features as shown above. The coefficient of variation was used for statistical feature selection. It was observed that the variation of the features was similar with the exception of two features (TSLM_stdev, and ESLM_stdev) which were dropped from all data sets resulting in 28 features.

Table S5:Feature coefficients of variation

Feature	CV = σ/μ
volt	0.0895
volt_mean	0.0326
volt_min	0.0608
volt_max	0.0469
volt_stdev	0.2084
volt_RMS	0.0325
rotation	0.1156
rotation_mean	0.0438
rotation_min	0.0852
rotation_max	0.0592
rotation_stdev	0.2106
rotation_RMS	0.0430
vibration	0.1369
vibration_mean	0.0656
vibration_min	0.1040
vibration_max	0.0787
vibration_stdev	0.2214
vibration_RMS	0.0652
TSLM	1.0933
TSLM_mean	1.0906
TSLM_min	1.1019
TSLM_max	1.0850
TSLM_stdev	9.3017
TSLM_RMS	1.0887
ESLM	1.0150
ESLM_mean	1.0112
ESLM_min	1.0221
ESLM_max	1.0051
ESLM_stdev	7.1235
ESLM_RMS	1.0088

10.4.4.2. Recursive Feature Elimination

After statistical feature selection, a recursive feature elimination algorithm was used for additional feature selection. A summary of the feature selection algorithm is shown below.

Figure S2: Overview of recursive feature elimination algorithm

Algorithm 2: Recursive feature elimination incorporating resampling

for *Each Resampling Iteration* **do**
    Partition data into training and test/hold–back set via resampling
    Tune/train the model on the training set using all predictors
    Predict the held–back samples
    Calculate variable importance or rankings
    for *Each subset size* S_i, $i = 1 \ldots S$ **do**
        Keep the S_i most important variables
        [Optional] Pre–process the data
        Tune/train the model on the training set using S_i predictors
        Predict the held–back samples
        [Optional] Recalculate the rankings for each predictor
    end
end
Calculate the performance profile over the S_i using the held–back samples
Determine the appropriate number of predictors
Estimate the final list of predictors to keep in the final model
Fit the final model based on the optimal S_i using the original training set

Source: R caret documentation

This algorithm was implemented using a random forest model with three repetitions of five-fold cross validation on each of the 168 data sets and default hyperparameters in R using the caret package. The selected features for each of the data sets are shown on the next two pages with black indicating that a feature was selected. It is observed that the number of features is fewer for each of the data sets, and this has the additional advantage of reduced training time.

Each of the 168 data sets was filtered by removing feature data of features that were not selected. This yielded 168 filtered data sets, each of which underwent further processing.

10.4.4.3. Selected Features

Table S6: Overview of selected features

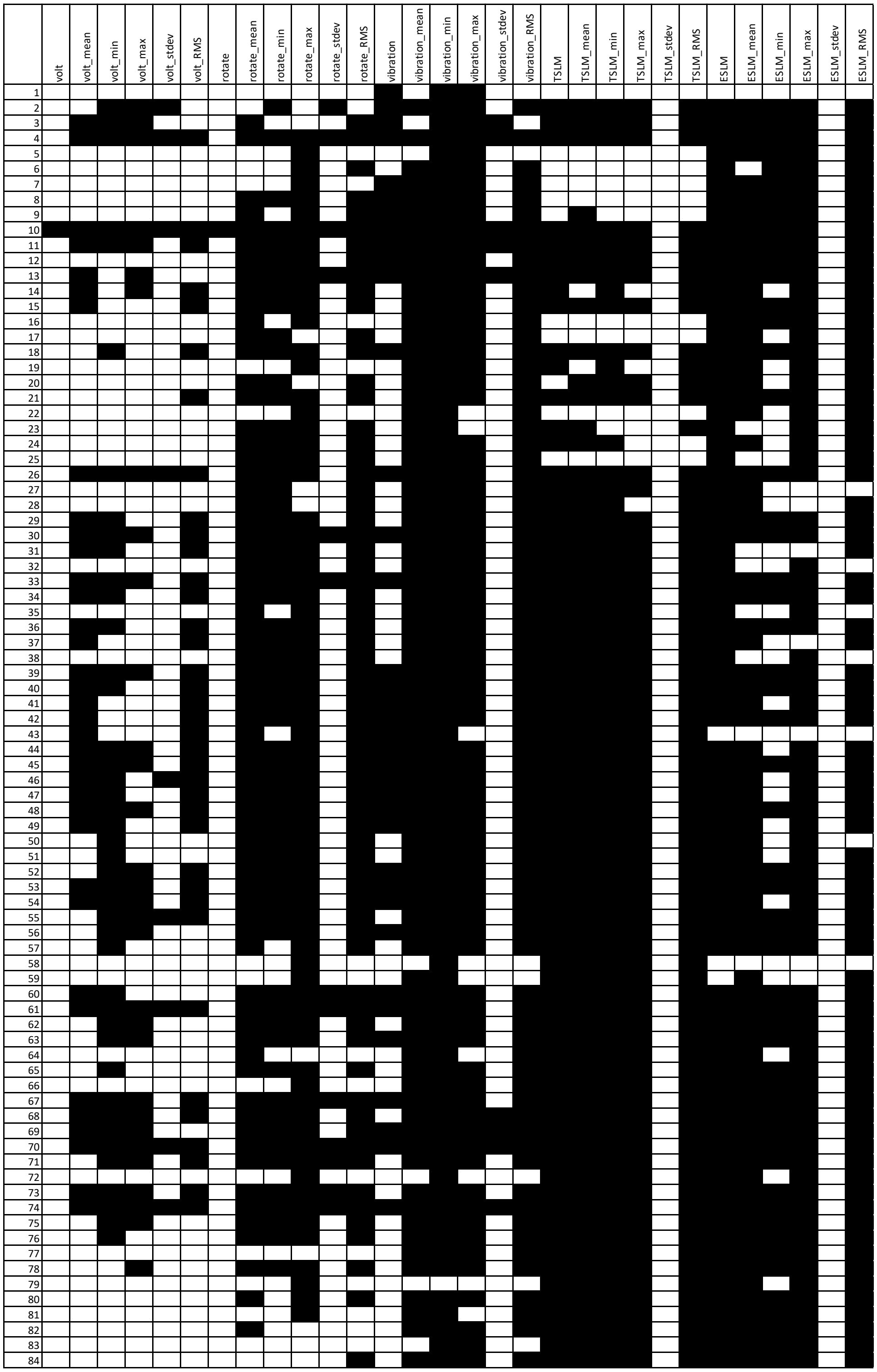


Table S6: Continued

	volt	volt_mean	volt_min	volt_max	volt_stdev	volt_RMS	rotate	rotate_mean	rotate_min	rotate_max	rotate_stdev	rotate_RMS	vibration	vibration_mean	vibration_min	vibration_max	vibration_stdev	vibration_RMS	TSLM	TSLM_mean	TSLM_min	TSLM_max	TSLM_stdev	TSLM_RMS	ESLM	ESLM_mean	ESLM_min	ESLM_max	ESLM_stdev	ESLM_RMS
85																														
86																														
87																														
88																														
89																														
90																														
91																														
92																														
93																														
94																														
95																														
96																														
97																														
98																														
99																														
100																														
101																														
102																														
103																														
104																														
105																														
106																														
107																														
108																														
109																														
110																														
111																														
112																														
113																														
114																														
115																														
116																														
117																														
118																														
119																														
120																														
121																														
122																														
123																														
124																														
125																														
126																														
127																														
128																														
129																														
130																														
131																														
132																														
133																														
134																														
135																														
136																														
137																														
138																														
139																														
140																														
141																														
142																														
143																														
144																														
145																														
146																														
147																														
148																														
149																														
150																														
151																														
152																														
153																														
154																														
155																														
156																														
157																														
158																														
159																														
160																														
161																														
162																														
163																														
164																														
165																														
166																														
167																														
168																														

10.4.5. Phase 3 – Balancing and Splitting

Red is used to indicate samples corresponding to failures, and green used to indicate samples that do not correspond to failures.

Figure S5: Overview of balancing and splitting

This phase yielded 168 pairs of training and validation sets. Each of the models was created using its corresponding training set, and evaluated using its corresponding validation set.

10.4.6. Phase 4 – Model Creation

Models were trained in R using caret. The algorithm used was nonlinear support vector machine classification with a radial basis function kernel. The hyperparameters C and σ were tuned on a grid produced by $441 = 21^2$ pairs of the following values $[2^{-10}, 2^{-9},\ldots,2^{9}, 2^{10}]$. This was done using 3 repetitions of 10-fold cross-validation. A total of 2,222,640 = 3*10*441*168 models were trained, however the overall output was one model with the best hyperparameters for each training set. As such, 168 models were created.

10.4.7. Phase 5 – Prediction

10.4.7.1. Overview

Three aspects of the future failure prediction approach that together help distinguish the methodology from other approaches are elucidated here. (1) ensemble creation, as opposed to using one model to predict future failure time, the present approach uses 12 models at a time as an ensemble of models to predict future failure; (2) p*robability threshold; t*he individual classification models output a probability of failure when applied, and an alarm is corresponds to an ensemble probability of failure exceeding a 99.999% threshold.; (3) *k-out-of-n alarm policy, t*his is further complemented with a 9-out-of-10 alarm policy in which a future failure is predicted if and only if there are 9 alarms triggered in a group of 10 ensembles.The three aspects of the failure prediction approach are illustrated with a table on a subsequent page. The output of the models is a future failure time of 129 hours corresponding to the first time the 9-out-of-10 policy is satisfied.

10.4.7.1. Model Evaluation Metrics

The metrics used to evaluate the performance of the models are defined here. The metrics involve true positives (TP), true negatives (TN), false positives (FP), false negatives (FN), probability of accurate agreement (p_1), and probability of chance agreement (p_2).

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{FP} + \text{TN} + \text{FN}}$$

$$\text{Kappa} = 1 - \frac{1 - p_1}{1 - p_2}$$

$$\text{Sensitivity} = \text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}$$

$$\text{Specificity} = \frac{\text{TN}}{\text{TN} + \text{FP}}$$

$$\text{F1} = \frac{2 * \text{Precision} * \text{Recall}}{\text{Precision} + \text{Recall}}$$

Table S7: Overview of individual and ensemble probabilities

Classifer	P_j^f	$1 - P_j^f$	P_e^f	P_e^f> 99.9999% ?	9-out-of-10 alarms ?
1	0.062913	0.937087	0.598066	No	No
2	0.131847	0.868153	0.607285	No	No
3	0.437723	0.562277	0.576630	No	No
4	0.029158	0.970842	0.248422	No	No
5	0.018865	0.981135	0.227404	No	No
6	0.025219	0.974781	0.213331	No	No
7	0.018498	0.981502	0.195388	No	No
8	0.021749	0.978251	0.180944	No	No
9	0.010804	0.989196	0.207781	No	No
10	0.002233	0.997767	0.202745	No	No
11	0.001085	0.998915	0.216976	No	No
12	0.000316	0.999684	0.217843	No	No
⋮	⋮	⋮	⋮	⋮	⋮
123	0.149036	0.850964	0.996355	No	No
124	0.325410	0.674590	0.999289	No	No
125	0.033409	0.966591	0.999124	No	No
126	0.091854	0.908146	0.999972	No	No
127	0.085693	0.914307	0.999994	No	No
128	0.075597	0.924403	0.999995	No	No
129	0.858849	0.141151	0.999999	Yes	Yes
130	0.445651	0.554349	0.999999	No	Yes
131	0.356005	0.643995	1.000000	Yes	Yes
132	0.453462	0.546538	1.000000	Yes	Yes
133	0.386458	0.613542	1.000000	Yes	Yes
134	0.493439	0.506561	1.000000	Yes	Yes
135	0.834096	0.165904	1.000000	Yes	Yes
136	0.168157	0.831843	1.000000	Yes	Yes
137	0.969376	0.030624	1.000000	Yes	Yes
138	0.812382	0.187618	1.000000	Yes	Yes
139	0.254292	0.745708	1.000000	Yes	Yes
140	0.868205	0.131795	1.000000	Yes	Yes
⋮	⋮	⋮	⋮	⋮	⋮

10.4.8. Phase 6 - Safety Quantification

A simplified safety metric is selected for the motivating example while a more complex one is selected for the second case study. The idea underlying the selected safety metric for the motivating example is that a reactor is less safe the closer it is to its maximum operating temperature is employed. This results in the following function which is input into the scheduling model.

$$(\mathbb{T}_t^U - \mathbb{T}_t) \geq \mathbb{T}_t^\Delta$$

10.4.9. Phase 7 – Scheduling

The model formulation is described in detail in the paper. Given that the models are relatively complex, additional pieces of information used for the implementation were: initializing the values of variables near the midpoint of their ranges, reformulating fractions as products where possible, and solving using an optimality gap threshold of 0.1 and time limit of 3600 s for both case studies.

The derivation of the pump switching constraints is presently described. A binary variable $s_{j,t}$ is defined to represent a switch in the status of a pump between two successive time periods for pumps $j \in J$ time periods $t \in T$. When there has been a switch, $s_{j,t} = 1$, when the pump status has remained off or remained on then $s_{j,t} = 0$. Defining propositions P_1 as pump 1 active in time t, P_2 as pump 2 active in time t + 1, and P_3 as a switch occurring, this can be represented using propositional logic as follows:

$$[\neg P_1 \wedge P_2] \vee [P_1 \wedge \neg P_2] \rightarrow P_3$$

$$[P_1 \wedge P_2] \vee [\neg P_1 \wedge \neg P_2] \rightarrow \neg P_3$$

Associating P_1 with $a_{j,t}$, P_2 with $a_{j,t+1}$, and P_3 with $s_{j,t}$, the following set of inequalities encoding the different possibilities can be defined:

$$s_{j,t} \leq a_{j,t} + a_{j,t+1}$$

$$s_{j,t} \geq a_{j,t+1} - a_{j,t}$$

$$s_{j,t} \geq a_{j,t} - a_{j,t+1}$$

$$s_{j,t} \leq 2 - a_{j,t} - a_{j,t+1}$$

The following constraint can then be defined to limit the number of switches over the time horizon for a given pump.

$$\sum_{t \in T} s_{j,t} \leq 1$$

10.5. Supporting Information for Chapter 6

10.5.1. Dynamic Simulation Model Examples

This section presents two examples of dynamic simulation models that were developed and then proceeds to provide additional information related to the multi-parametric-based safety-aware, maintenance-aware, and disruption-aware (mpSAMADA) framework.

10.5.1.1. Dynamic Simulation of a Continuous Production Process

The selected continuous process involves the production of methyl acetate in a homogenous liquid medium and was taken from a gPROMS tutorial. Methanol (MeOH) and acetic acid (HAc) are combined in a continuous stirred tank reactor (CSTR) to form methyl acetate (MeAc) and water (H_2O). There are two reactions (1) a forward esterification reaction, and (2) a reverse hydrolysis reaction. This is shown below:

$$\mathrm{CH_3OH + CH_3COOH \rightleftharpoons CH_3COOCH_3 + H_2O}$$

This motivating example illustrates the dynamic operation of a well-stirred isothermal continuous production system. The initial liquid level in the reactor is 2 m and the outlet line is located at a height of 5 m. Reactants are fed in causing the level to rise and products to be formed, and the system exhibits a state transition once the liquid level reaches the outlet line level.

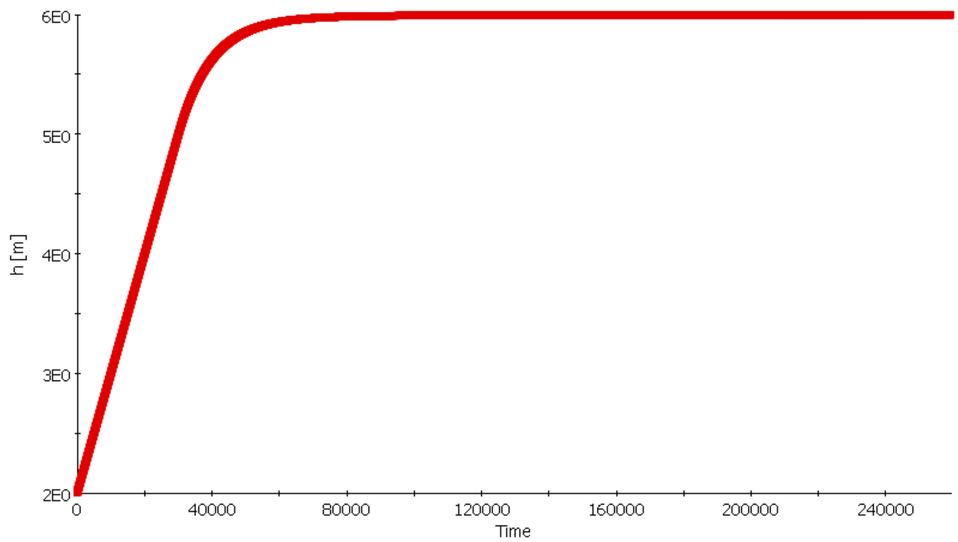


Figure S6: CSTR liquid level

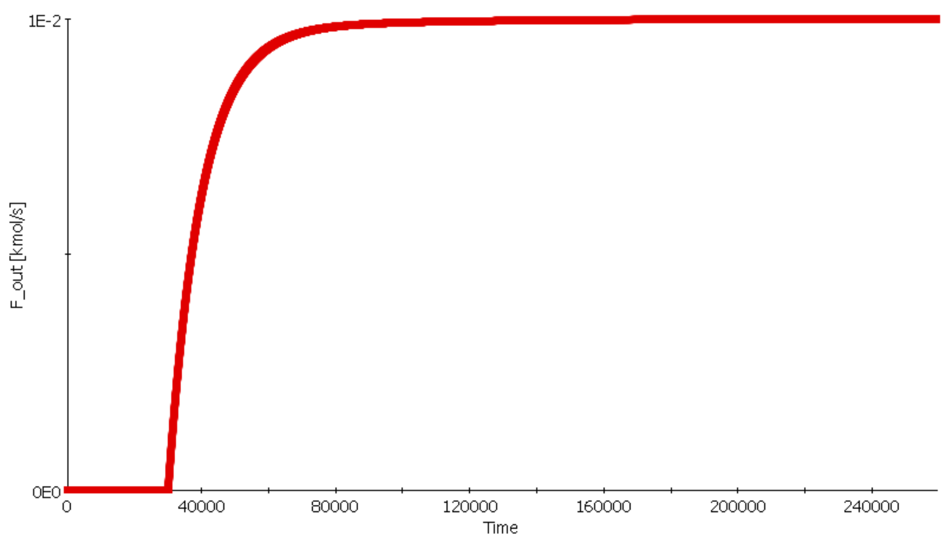


Figure S7: CSTR outlet flowrate

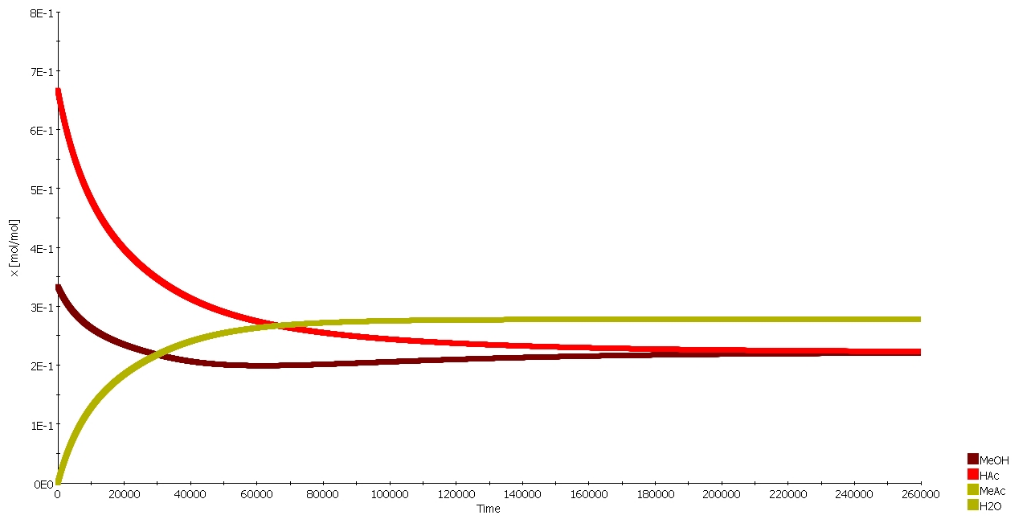


Figure S8: CSTR species compositions

10.5.1.2. Dynamic Simulation of a Multi-Product Batch Production Process

The selected batch process involves a multiproduct batch plant with a mixing stage and a reaction stage and was adapted from [187] and a gPROMS tutorial. The process is a fed batch process in which one set of chemical species is mixed in one tank, and a second set of chemical species is mixed in a second tank before being fed to a reactor. Modeling considerations include perfect mixing, limited reaction in the mixing tanks, isothermal process behavior, and controlled outlet flowrates from the mixing tanks once the outlet valves are opened. An overview of the operating procedures and system states is provided.

This motivating example captures more complex operating procedures such as sequential feeds, and the influence of valve control. This enables the elucidation of process and maintenance scheduling as well as fault prediction. In particular, equipment faults such as valve stiction or agitator failure can lead to a process fault, and this can be captured through a fault prediction model and then used to obtain maintenance-aware fault-aware optimal predictive control strategies.

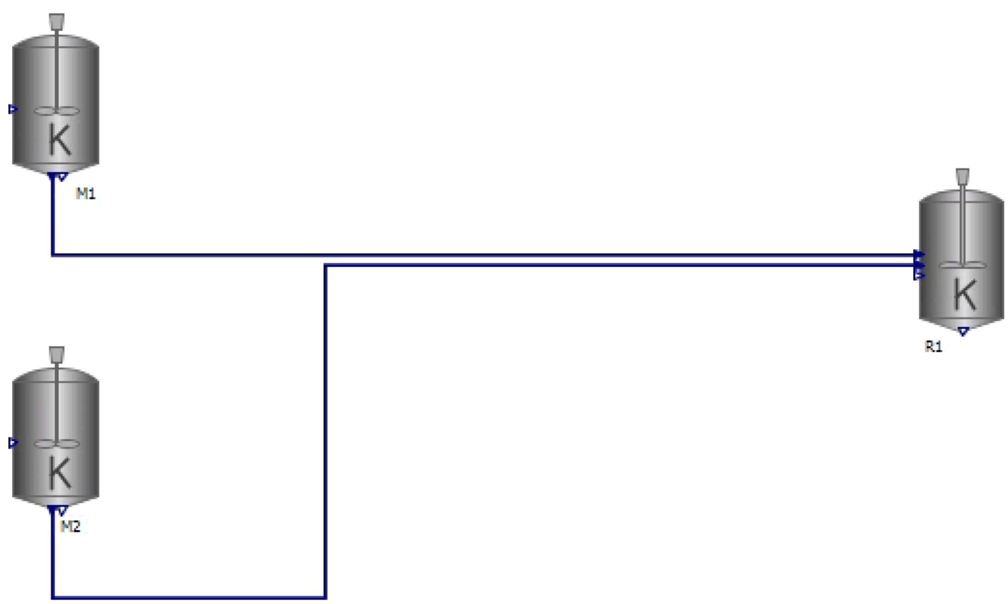


Figure S8: Multi-product batch process flowsheet

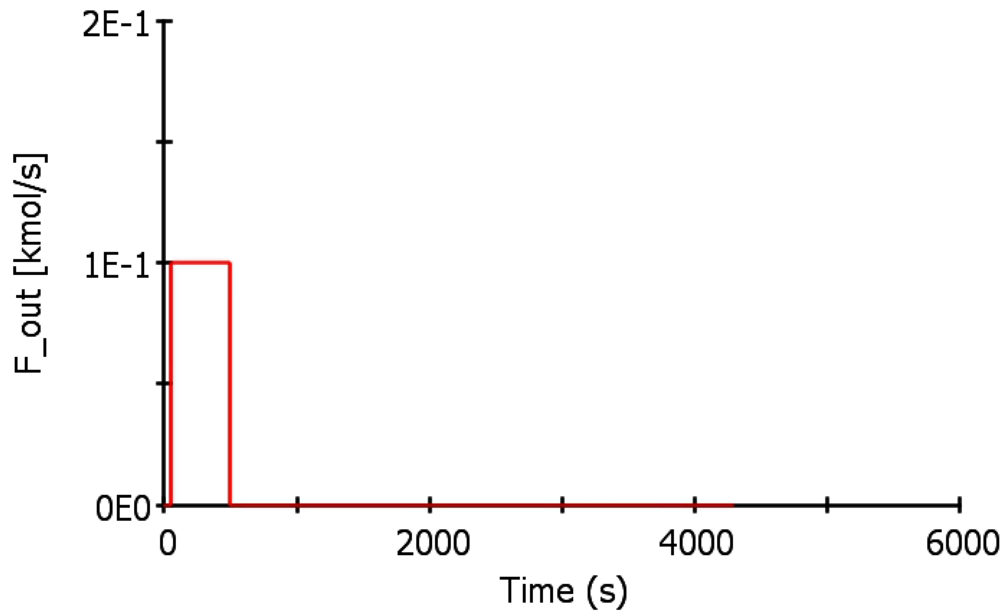


Figure S9: Primary mixing tank outlet flowrate

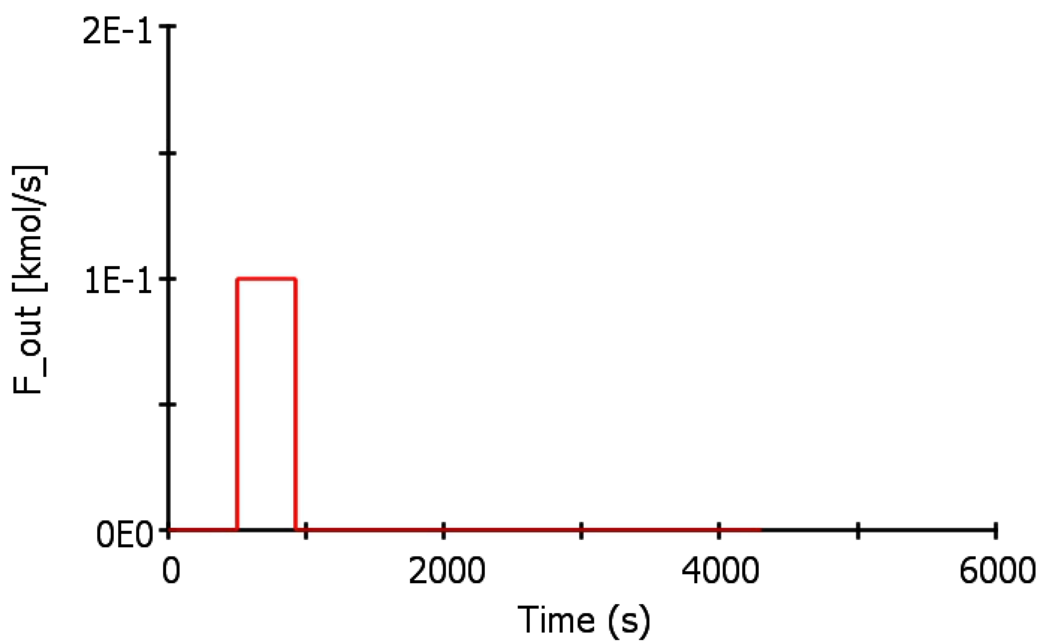


Figure S10: Secondary mixing tank outlet flowrate

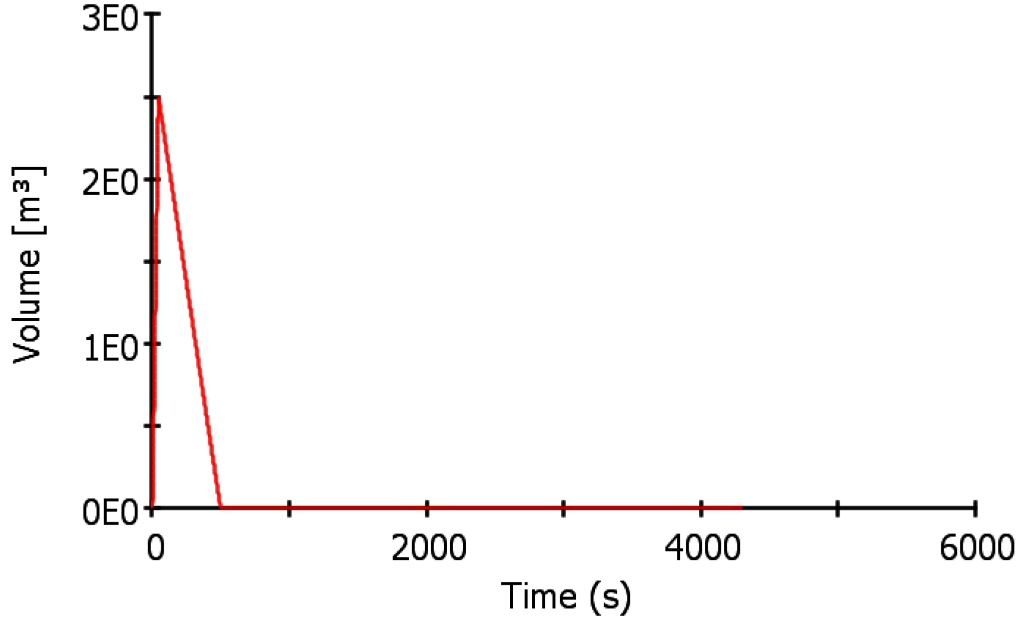


Figure S11: Primary mixing tank volume

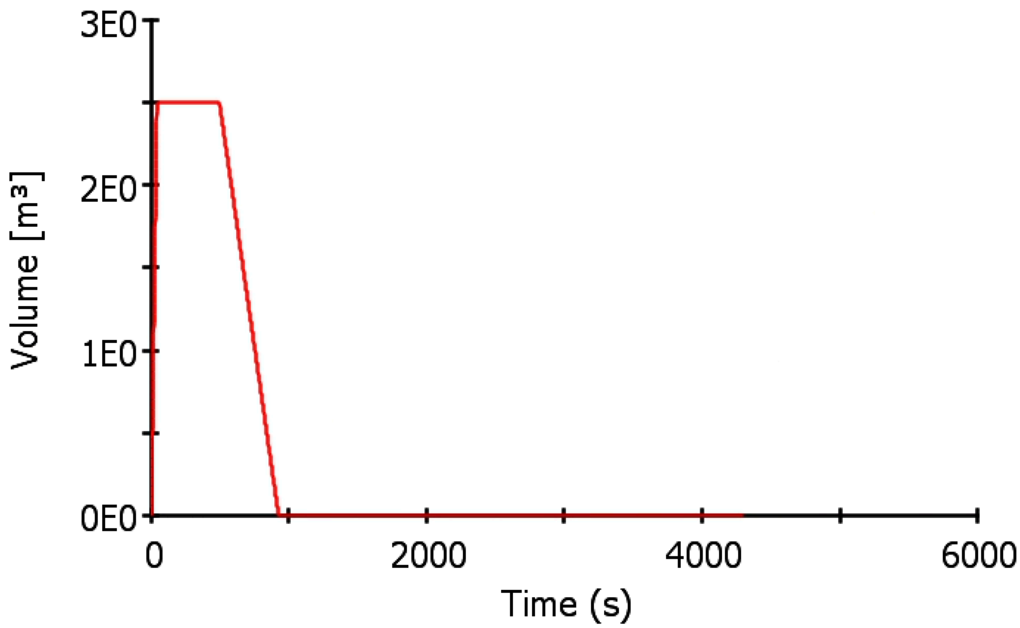


Figure S12: Secondary mixing tank volume

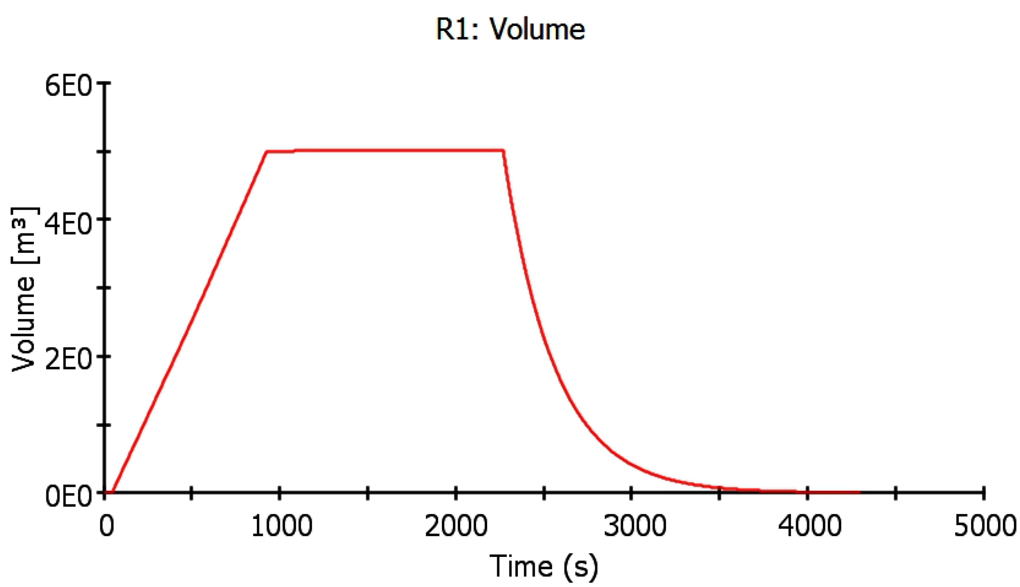


Figure S13: Batch reactor volume

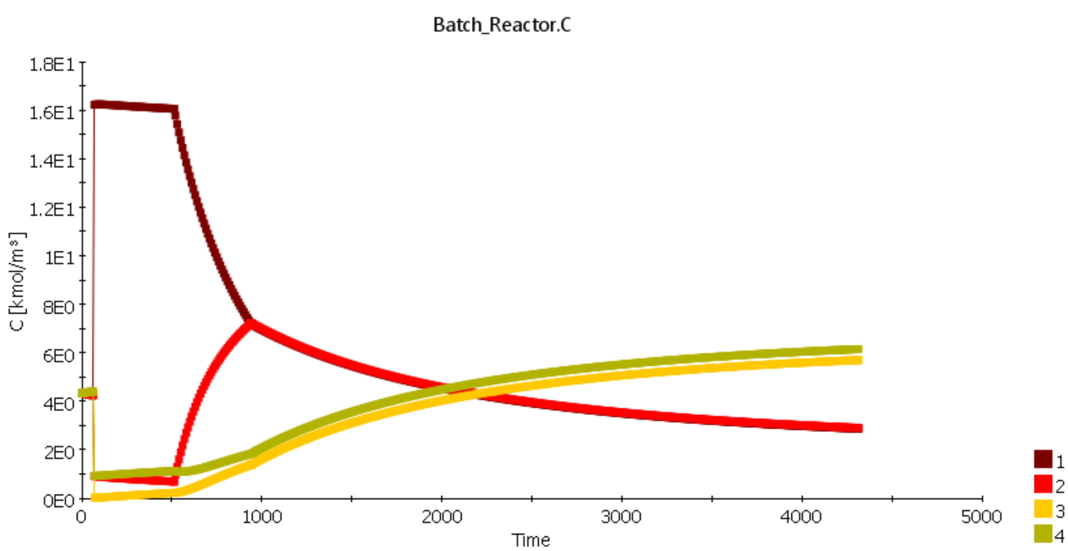


Figure S14: Batch reactor species concentrations

10.5.2. Case Study 1 – System Reliability Function Derivation

The overall system can be iteratively subdivided into subsystems A, B, and C such that $R_A = f(R_1, R_2)$, $R_B = f(R_A, R_3)$, $R_C = f(R_4)$, and $R^{sys} = f(R_B, R_C)$.

$$R^{series} = \prod_{j \in J^{series}} R_j$$

$$R^{parallel} = 1 - \prod_{j \in J^{parallel}} \left(1 - R_j\right)$$

For two components, $R^{series} = R_1 R_2$ and $R^{parallel} = R_1 + R_2 - R_1 R_2$. The system reliability function can thus be determined.

$$R_A = R_1 + R_2 - R_1 R_2$$

$$R_B = R_A R_3 = R_1 R_3 + R_2 R_3 - R_1 R_2 R_3$$

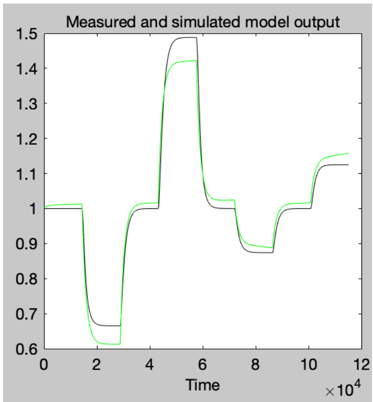
$$R_C = R_4$$

$$R^{sys} = R_B + R_C - R_B R_C$$

$$R^{sys} = R_1 R_3 + R_2 R_3 - R_1 R_2 R_3 + R_4 + R_1 R_3 R_4 - R_2 R_3 R_4 + R_1 R_2 R_3 R_4$$

10.5.3. Case Study 1 – Model Approximation

(a)



(b)

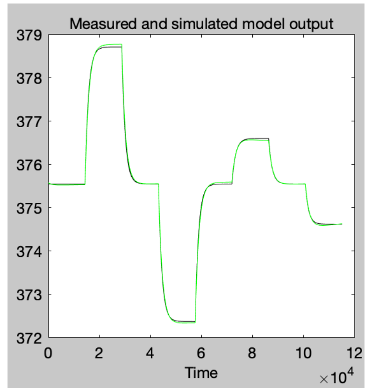


Figure S15: Case Study 1 – Model approximation for state space model with disturbances (a) concentration, and (b) temperature

10.5.4. Case Study 1 – State-Space Model Matrices

$$A = \begin{bmatrix} 1 & 2.433e^{-4} \\ 8.579e^{-5} & 0.999 \end{bmatrix}$$

$$B = \begin{bmatrix} 8.320e^{-7} \\ -2.255e^{-6} \end{bmatrix}$$

$$C = \begin{bmatrix} -1.312e^{-6} \\ 3.518e^{-6} \end{bmatrix}$$

$$D = \begin{bmatrix} -66.516 & 0.0446 \\ -314.049 & -314.243 \end{bmatrix}$$

10.5.5. Case Study 1 – mpMPC Model and Tuning Parameters

$$\min_{u} \sum_{k=1}^{OH-1} y_k^T QR_k y_k^T$$

$$s.t. x_{k+1} = Ax_k + Bu_k + Cd_k$$

$$y_k = Dx_k$$

$$u_{min} \leq u_k \leq u_{max}$$

$$\Delta u_{min} \leq \Delta u_k \leq \Delta u_{max}$$

$$x_{min} \leq x_k \leq x_{max}$$

$$y_{min} \leq y_k \leq y_{max}$$

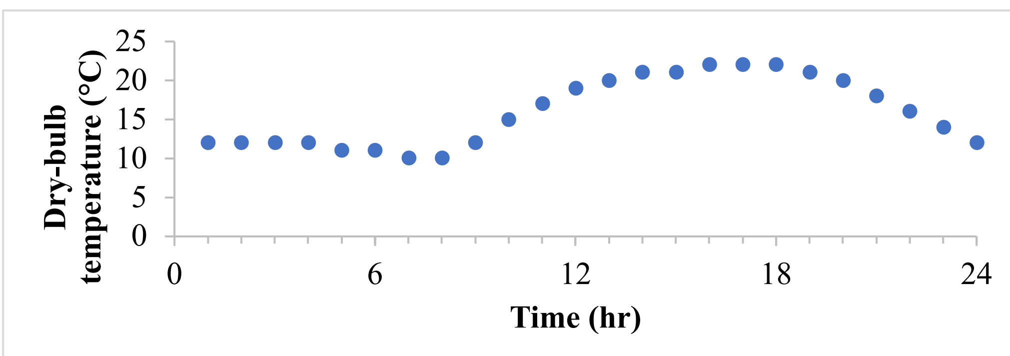
Table S8: Case Study 1 - Tuning parameters of the mpMPC controller

Parameter	Value
OH	5
NC	1
QR	10^4
u_{min}	350
u_{max}	370
Δu_{min}	-0.01
Δu_{max}	0.01
x_{min}	$[-1 \quad -2]^T$
x_{max}	$[0 \quad 0]^T$
y_{min}	$[0 \quad 300]^T$
y_{max}	$[0 \quad 500]^T$

10.5.1. Case Study 2 – Air Temperature and Humidity Profiles

The second case study used the approximate air temperature and humidity profiles for Kingsport, TN, USA on Apr 6th, 2020. American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE) formulas were used on https://www.kwangu.com/work/psychrometric.htm to calculate the corresponding wet-bulb temperatures.

(a)



(b)

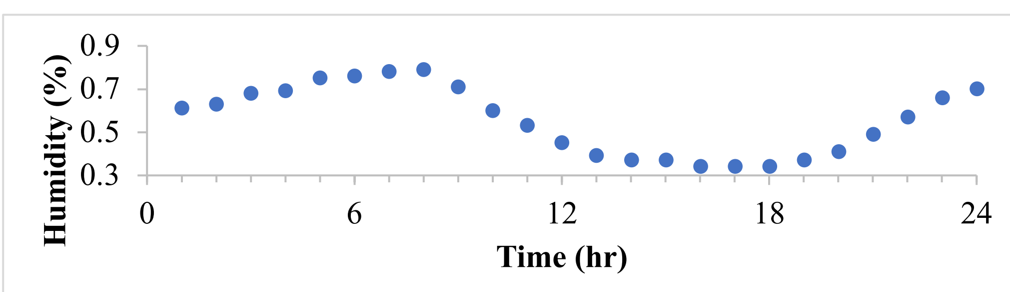


Figure S16: Profiles of (a) air temperature, and (b) humidity

10.5.2. Case Study 2 – Scheduling

The monolithic process and maintenance scheduling model was computationally demanding so it was solved by formulating it as two problems: (1) a cooling tower scheduling problem, and (2) a pump network problem. The cooling tower model was adapted from previous work in the literature.

10.5.2.1. *C*ooling Tower Model

Sets:

- time intervals, $t \in T$

Continuous Variables*:*

- air flowrate (m_t^{air})
- inlet air wet-bulb temperature ($T_t^{air,wb,in}$)
- inlet water temperature ($T^{w,in}$)
- inlet vapor pressure ($P_t^{vap,wb,in}$)
- inlet air-vapor flowrate ($m_t^{av,in}$)
- inlet air water mass fraction (w_t^{in})
- inlet air density (ρ_t^{air})
- inlet air enthalpy ($h^{air,in}$)
- mean air-vapor flowrate ($m_t^{av,m}$)
- mean air density ($\rho_t^{air,m}$)
- mass flowrate of evaporated water (m_t^{wev})
- mass of makeup water (m_t^{mw})

- outlet water temperature ($T_t^{w,out}$)
- outlet air water mass fraction (w_t^{out})
- outlet air temperature ($T_t^{air,out}$)
- outlet air-vapor flowrate ($m_t^{av,out}$)
- outlet air density (ρ_t^{air})
- outlet vapor pressure ($P^{vap,out}$)
- power (P_t)
- pressure difference (ΔP_t)
- miscellaneous pressure difference (ΔP_t^{misc})
- pressure difference due to fills (ΔP_t^{fi})
- saturated air enthalpy (h_t^{sa})
- water flowrate (m_t^{w})

$$\min \sum_{t \in T} c^w 3600 m_t^{mw} + c^e \left(\frac{P^t}{1000}\right) \tag{173}$$

$$\begin{aligned} P_t^{vap,wb,in} = {} & 0.0009023831\left(T_t^{air,wb,in}\right)^4 - 0.0260853788\left(T_t^{air,wb,in}\right)^3 \\ & + 3.4738430795\left(T_t^{air,wb,in}\right)^2 \\ & + 9.2228935076 T_t^{air,wb,in} + 822.0620060852 \end{aligned} \qquad t \in T \tag{174}$$

$$\begin{aligned} w_t^{in} = {} & \left(\frac{2501.6 - 2.3263 T_t^{wb,in}}{2506 + 1.8577 T_t^{air,in} - 4.184 T_t^{wb,in}}\right)\left(\frac{0.62509 P_t^{vap,wb,in}}{P^{tot} - 1.005 P_t^{vap,wb,in}}\right) \\ & - \left(\frac{1.00416(T_t^{air,in} - T_t^{wb,in})}{2506 + 1.8577 T_t^{air,in} - 4.184 T_t^{wb,in}}\right) \end{aligned} \qquad t \in T \tag{175}$$

$$\rho_t^{air,in} = \frac{P^{tot}}{287.08 T_t^{air,in} + 273.15}\left(1 - \frac{w_t^{air,in}}{w_t^{air,in} + 0.62198}\right)\left(1 + w_t^{air,in}\right) \qquad t \in T \tag{176}$$

$$\begin{aligned} h^{air,in} = {} & -6.38887667 + 0.86581791 T^{water,in} \\ & + 15.7153617 e^{0.0543977 T^{water,in}} \end{aligned} \qquad t \in T \tag{177}$$

$$m_t^{mw} = \frac{n^{cycles}}{n^{cycles} - 1} m_t^{wev} \qquad t \in T \tag{178}$$

$$m_t^{wev} = m_t^{air}(w_t^{out} - w_t^{in}) \qquad t \in T \quad (179)$$

$$w_t^{out} = \frac{0.62509 P_t^{vap,out}}{P^{tot}} \qquad t \in T \quad (180)$$

$$P_t^{vap,out} = 0.0009023831\left(T_t^{air,out}\right)^4 - 0.0260853788\left(T_t^{air,out}\right)^3 + 3.4738430795\left(T_t^{air,out}\right)^2 + 9.2228935076 T_t^{air,out} + 822.0620060852 \qquad t \in T \quad (181)$$

$$h_t^{sa} = h^{air,in} + \frac{C_p^w m_t^w}{m_t^{air}}\left(T^{water,in} - T_t^{water,out}\right) \qquad t \in T \quad (182)$$

$$T_t^{water,out} = T^{water,D} \qquad t \in T \quad (183)$$

$$P_t = \frac{m_t^{av,in} \Delta P_t}{\rho_t^{air,in} \eta_f} \qquad t \in T \quad (184)$$

$$\Delta P_t = 1.667(\Delta P_t^{fi} + \Delta P_t^{misc}) \qquad t \in T \quad (185)$$

$$\Delta P_t^{fi} = K_{fi} L_{fi} \frac{(m_t^{av,m})^2}{2\rho_t^{air,m}(A^{fr})^2} \qquad t \in T \quad (186)$$

$$\Delta P_t^{misc} = 6.5 \frac{(m_t^{av,m})^2}{2\rho_t^{air,m}(A^{fr})^2} \qquad t \in T \quad (187)$$

$$m_t^{av,m} = \frac{m_t^{av,in} + m_t^{av,out}}{2} \qquad t \in T \quad (188)$$

$$m_t^{av,in} = m_t^{air} + w_t^{in} m_t^{air} \qquad t \in T \quad (189)$$

$$m_t^{av,out} = m_t^{air} + w_t^{out} m_t^{air} \qquad t \in T \quad (190)$$

$$\frac{1}{\rho_t^{air,m}} = \frac{1}{\rho_t^{air,in}} + \frac{1}{\rho_t^{air,out}} \qquad t \in T \quad (191)$$

$$\rho_t^{air,out} = \frac{P^{tot}}{287.08 T_t^{air,in} + 273.15}\left(1 - \frac{w_t^{air,out}}{w_t^{air,out} + 0.62198}\right)\left(1 + w_t^{air,out}\right) \qquad t \in T \quad (192)$$

$$1.2 \leq \frac{m_t^{air}}{A^{fr}} \leq 4.25 \qquad t \in T \quad (193)$$

$$2.9 \leq \frac{m_t^{w}}{A^{fr}} \leq 5.96 \qquad t \in T \quad (194)$$

$$0.5 \leq \frac{m_t^w}{m_t^{air}} \leq 2.5 \qquad t \in T \quad (195)$$

$$T_t^{air,out} \geq T_t^{air,in} \qquad t \in T \quad (196)$$

$$T^{water,in} \geq T^{water,out} \qquad t \in T \quad (197)$$

$$T^{water,out} \geq 2.8 + T^{air,wb,in} \qquad t \in T \quad (198)$$

$$m_t^{mw} \geq 0.01 m_t^w \qquad t \in T \quad (199)$$

10.5.2.2. Pump Network Model

Sets:

- pumps, $j \in J$
- streams, $s \in S$
- time intervals, $t \in T$
- miscellaneous time intervals $t \in T^1$, $t \in T^2$, $t \in T^3$, $t \in T^4$, $t \in T^5$

Continuous Variables:

- predicted pump reliability ($R_{j,t}^{pred}$)
- pump efficiency ($\eta_{j,t}$)
- pump power ($P_{j,t}^{pump}$),

Binary Variables:

- availability ($a_{j,t}$)
- maintenance ($m_{j,t}$)
- prior maintenance ($m_{j,t}^{prior}$)
- started maintenance ($m_{j,t}^{start}$)
- switch ($\sigma_{j,t}$)

$$\min \sum_{t\in T}\left[c^{e}\sum_{j\in J}P_{j,t}^{pump}+\left(1-R_{1,t}^{pred}\right)c^{m}m_{1,t}\right] \tag{200}$$

$$F_{2,t}=F^{S} \qquad t\in T \tag{201}$$

$$F_{2,t}=F_{3,t}+F_{9,t} \qquad t\in T \tag{202}$$

$$F_{3,t}=F_{4,t}+F_{5,t} \qquad t\in T \tag{203}$$

$$F_{4,t}=F_{6,t} \qquad t\in T \tag{204}$$

$$F_{5,t}=F_{7,t} \qquad t\in T \tag{205}$$

$$F_{6,t}+F_{7,t}=F_{8,t} \qquad t\in T \tag{206}$$

$$F_{9,t}=F_{10,t} \qquad t\in T \tag{207}$$

$$F_{8,t}+F_{10,t}=F_{11,t} \qquad t\in T \tag{208}$$

$$\eta_{1,t}=\gamma_1\left(F_{6,t}\right)^2+\gamma_2F_{6,t}+\gamma_3 \qquad t\in T \tag{209}$$

$$\eta_{2,t}=\gamma_1\left(F_{7,t}\right)^2+\gamma_2F_{7,t}+\gamma_3 \qquad t\in T \tag{210}$$

$$\eta_{3,t}=\gamma_1\left(F_{10,t}\right)^2+\gamma_2F_{10,t}+\gamma_3 \qquad t\in T \tag{211}$$

$$P_{1,t}^{pump}=\frac{F_{6,t}\rho gH}{\chi\eta_{1,t}} \qquad t\in T \tag{212}$$

$$P_{2,t}^{pump}=\frac{F_{7,t}\rho gH}{\chi\eta_{2,t}} \qquad t\in T \tag{213}$$

$$P_{3,t}^{pump}=\frac{F_{10,t}\rho gH}{\chi\eta_{3,t}} \qquad t\in T \tag{214}$$

$$a_{1,t}F_1^L\le F_{6,t}\le a_{1,t}F_1^U \qquad t\in T \tag{215}$$

$$a_{2,t}F_2^L\le F_{7,t}\le a_{2,t}F_2^U \qquad t\in T \tag{216}$$

$$a_{3,t}F_3^L\le F_{10,t}\le a_{3,t}F_3^U \qquad t\in T \tag{217}$$

$$1-a_{j,t}\ge m_{j,t} \qquad t\in T \tag{218}$$

$$\sum_{t\in T^1} m_{1,t}^{start} = 1 \quad (219)$$

$$\sum_{j\in J} m_{j,t} \leq 1 \qquad t \in T \quad (220)$$

$$\sum_{\tau\in T^2} m_{j,\tau} \geq MTTR_j m_{j,t}^{start} \qquad t \in T^3\ \forall j \in J^1 \quad (221)$$

$$\sum_{t\in T} m_{j,t} \leq MTTR_j \qquad t \in T\ \forall j \in J^1 \quad (222)$$

$$\sigma_{j,t} \leq a_{j,t} + a_{j,t+1} \quad (223)$$

$$\sigma_{j,t} \geq a_{j,t+1} - a_{j,t} \quad (224)$$

$$\sigma_{j,t} \geq a_{j,t} - a_{j,t+1} \quad (225)$$

$$\sigma_{j,t} \leq 2 - a_{j,t} - a_{j,t+1} \quad (226)$$

$$\sum_{t\in T} \sigma_{j,t} \leq \kappa_j^s \qquad t \in T\ j \in J \quad (227)$$

$$m_{1,t+1}^{prior} \geq m_{1,t}^{start} \qquad \forall t \in T^4 \quad (228)$$

$$m_{1,t+1}^{prior} \geq m_{1,t}^{prior} \qquad \forall t \in T^4 \quad (229)$$

$$\sum_{\tau\in T_t^5} m_{1,\tau}^{start} \geq m_{1,t+1}^{prior} \qquad t \in T^4 \quad (230)$$

$$R_{1,t}^{pred} = 1 - \frac{1}{1 + e^{-\lambda_1(t-\lambda_2)}} \qquad t \in T \quad (231)$$

$$R_{1,t} = R_{1,t}^{pred}\left(1 - m_{1,t}^{prior}\right) + (1)m_{1,t}^{prior} \qquad t \in T \quad (232)$$

10.5.3. Case Study 2 - Features

Table S9: Case Study 2 – List of features

Feature	Description		Feature	Description
F1	A Feed Flowrate		F27	Composition of E in Reactor Feed
F2	D Feed Flowrate		F28	Composition of F in Reactor Feed
F3	E Feed Flowrate		F29	Composition of A in Purge Feed
F4	Total Feed Flowrate		F30	Composition of B in Purge Feed
F5	Recycle Flowrate		F31	Composition of C in Purge Feed
F6	Reactor Feed Flowrate		F32	Composition of D in Purge Feed
F7	Reactor Pressure		F33	Composition of E in Purge Feed
F8	Reactor Level		F34	Composition of F in Purge Feed
F9	Reactor Temperature		F35	Composition of G in Purge Feed
F10	Purge Flowrate		F36	Composition of H in Purge Feed
F11	Product Separator Temperature		F37	Composition of D in Product Stream
F12	Product Separator Level		F38	Composition of E in Product Stream
F13	Product Separator Pressure		F39	Composition of F in Product Stream
F14	Product Separator Underflow Flowrate		F40	Composition of G in Product Stream
F15	Stripper Level		F41	Composition of H in Product Stream
F16	Stripper Pressure		F42	Feed Flowrate of D
F17	Stripper Underflow Flowrate		F43	Feed Flowrate of E
F18	Stripper Temperature		F44	Feed Flowrate of A
F19	Stripper Stream Flow		F45	Total Feed Flowrate
F20	Compressor Work		F46	Compressor Recycle Valve Position
F21	Reactor Cooling Water Outlet Temperature		F47	Purge Valve Position
F22	Separator Cooling Water Outlet Temperature		F48	Separator Pot Liquid Flowrate
F23	Composition of A in Reactor Feed		F49	Stripper Liquid Product Flowrate
F24	Composition of B in Reactor Feed		F50	Stripper Steam Valve Position
F25	Composition of C in Reactor Feed		F51	Reactor Cooling Water Flowrate
F26	Composition of D in Reactor Feed		F52	Condenser Cooling Water Flowrate

10.5.4. Model Evaluation Metrics

The metrics used to evaluate the performance of the models are defined here. The metrics involve true positives (TP), true negatives (TN), false positives (FP), false negatives (FN).

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{FP} + \text{TN} + \text{FN}}$$

$$\text{Sensitivity} = \text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

$$\text{Specificity} = \frac{\text{TN}}{\text{TN} + \text{FP}}$$

10.5.5. Recursive Feature Elimination Algorithm

A summary of the feature selection algorithm is shown below and has been taken from the R caret documentation.

Algorithm S1: Overview of recursive feature elimination algorithm

Algorithm 2: Recursive feature elimination incorporating resampling

```
for Each Resampling Iteration do
    Partition data into training and test/hold–back set via resampling
    Tune/train the model on the training set using all predictors
    Predict the held–back samples
    Calculate variable importance or rankings
    for Each subset size S_i, i = 1...S do
        Keep the S_i most important variables
        [Optional] Pre–process the data
        Tune/train the model on the training set using S_i predictors
        Predict the held–back samples
        [Optional] Recalculate the rankings for each predictor
    end
end
Calculate the performance profile over the S_i using the held–back samples
Determine the appropriate number of predictors
Estimate the final list of predictors to keep in the final model
Fit the final model based on the optimal S_i using the original training set
```

Table S10: Case Study 2 – Feature importance values

Feature	Importance		Feature	Importance
F1	2.55		F27	3.92
F2	1.52		F28	5.01
F3	3.27		F29	3.68
F4	0.70		F30	2.84
F5	0.45		F31	3.57
F6	1.06		F32	2.25
F7	6.64		F33	3.69
F8	0.96		F34	3.71
F9	28.47		F35	3.63
F10	2.98		F36	2.82
F11	2.87		F37	5.74
F12	1.06		F38	7.61
F13	6.62		F39	6.21
F14	0.12		F40	5.52
F15	1.60		F41	7.94
F16	5.34		F42	1.03
F17	0.77		F43	1.60
F18	7.02		F44	2.42
F19	5.82		F45	0.64
F20	7.50		F46	4.55
F21	27.73		F47	2.33
F22	0.44		F48	0.66
F23	2.30		F49	1.59
F24	2.67		F50	6.48
F25	3.34		F51	28.17
F26	2.90		F52	0.91

10.5.6. Case Study 2 – Model Creation Training Details

The data was used to create three classification models to label samples of data as being either normal or faulty. A summary of the implementation details for each algorithm is provided here. It is noted that the illustrations of each algorithm do not necessarily correspond to the fault detection decision logic.

10.5.6.1. Artificial Neural Network Model (ANN)

The ANN model was built on the training data with 5 repeats of 10-fold cross-validation and has a 3/5/2 structure. Rectified linear unit (ReLU) and softmax were used as activation functions for the hidden layer and output layer nodes respectively. Training was done to optimize cross-entropy via stochastic gradient descent with the hyperparameter lr = 0.01.

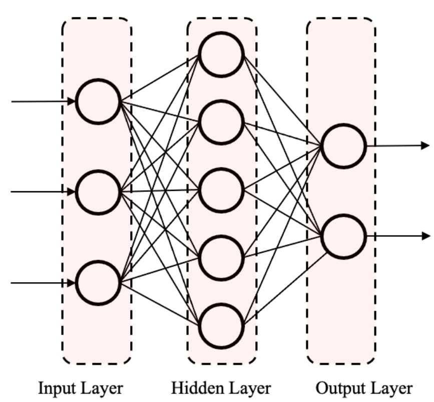


Figure S17: Generalized ANN depiction

10.5.6.2. Decision Tree (DT)

The DT was built on the training data with 5 repeats of 10-fold cross-validation and a complexity hyperparameter of 0.01.

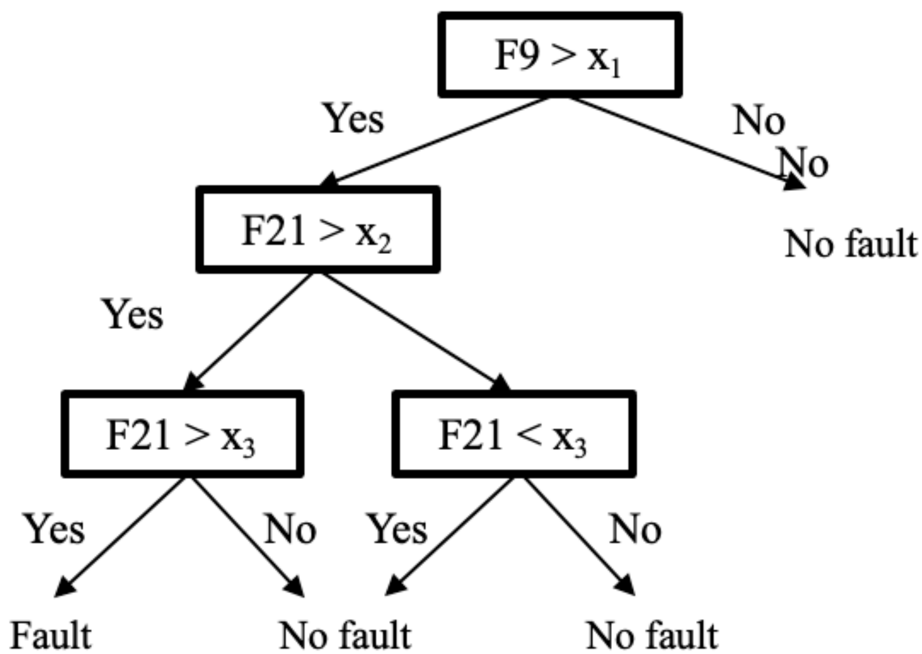


Figure S18: Generalized DT depiction

10.5.6.3. Support Vector Machine (SVM)

The SVM was built on the training data with 5 repeats of 10-fold cross-validation. The cost-sensitive weight factor used was 1.041667.The radial basis function was used as the kernel and hyperparameters σ and C were trained on a [2^{-10}, 2^{10}] grid.

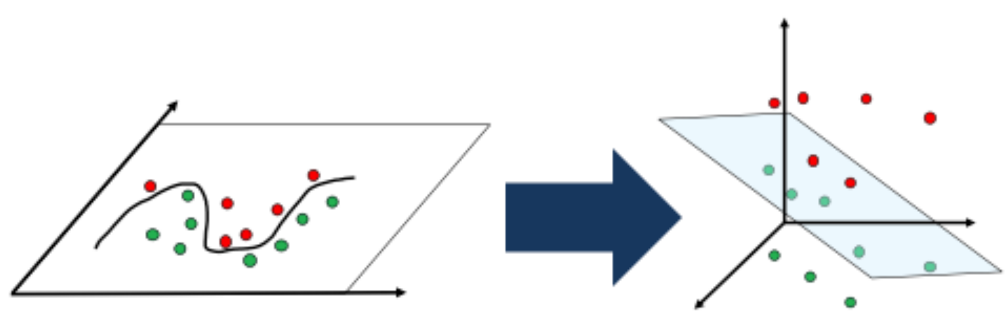


Figure S19: Generalized SVM depiction

10.5.7. Case Study 2 – High-Fidelity Model

$$\frac{dM^{basin}}{dt} = m^{basin,in} - m^{out} + m^{makeup} - m^{evap}$$

$$m^{evap} = m^{air}(w^{out} - w^{in})$$

$$w^{in} = \frac{0.62509P^{vap,wb,in}}{P_{tot} - 1.05P^{vap,wb,in}}$$

$$w^{exit} = \frac{0.62509P^{exit}}{P_{tot} - 1.05P^{exit}}$$

$$P_t^{vap,wb,in} = 0.0009023831\left(T_t^{air,wb,in}\right)^4 - 0.0260853788\left(T_t^{air,wb,in}\right)^3 + 3.4738430795\left(T_t^{air,wb,in}\right)^2 + 9.2228935076T_t^{air,wb,in} + 822.0620060852$$

$$P_t^{vap,out} = 0.0009023831\left(T_t^{air,out}\right)^4 - 0.0260853788\left(T_t^{air,out}\right)^3 + 3.4738430795\left(T_t^{air,out}\right)^2 + 9.2228935076T_t^{air,out} + 822.0620060852$$

$$m^{makeup} = m^{evap}$$

$$m_{out} = \rho^w Q_1 + \rho^w Q_2 + \rho^w Q_3$$

$$\omega_1 = \frac{Q_1}{Q^{nom}}\omega^{nom}$$

$$\omega_2 = \frac{Q_2}{Q^{nom}}\omega^{nom}$$

$$\omega_3 = \frac{Q_3}{Q^{nom}} \omega^{nom}$$

$$\eta_1 = \beta_1 Q_1^4 + \beta_2 Q_1^3 + \beta_3 Q_1^2 + \beta_4 Q_1 + \beta_5$$

$$\eta_2 = \beta_1 Q_2^4 + \beta_2 Q_2^3 + \beta_3 Q_2^2 + \beta_4 Q_2 + \beta_5$$

$$\eta_3 = \beta_1 Q_3^4 + \beta_2 Q_3^3 + \beta_3 Q_3^2 + \beta_4 Q_3 + \beta_5$$

$$Q = Q_1 + Q_2 + Q_3$$

Table S11: Case Study 2 – High-fidelity model parameters

Parameter	Symbol	Value
Ambient pressure, Pa	P^{tot}	101325
Density of water, kg/m^3	ρ^w	1000
Inlet air dry-bulb temperature, °C	$T^{air,in}$	17
Inlet air wet-bulb temperature, °C	$T^{air,wb,in}$	12
Nominal pump 1 rotational speed, RPM	ω_1	2407
Nominal pump 1 rotational speed, RPM	ω_2	2407
Nominal pump 1 rotational speed, RPM	ω_3	2407
Reference rotational speed, RPM	ω^{nom}	2900
Reference flowrate, m^3/hr	Q^{nom}	35.5
Number of cycles	n^{cycles}	4

10.5.8. Case Study 2 – Model Approximation

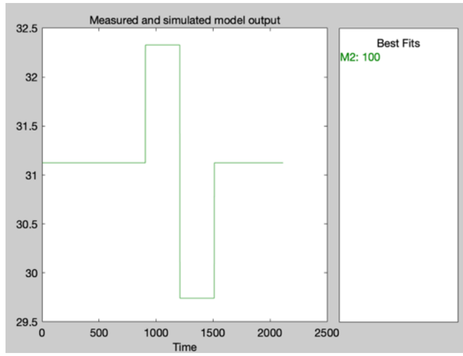


Figure S20: Model approximation for state-space model

10.5.9. Case Study 2 – State-Space Model and State-Space Model Matrices

$$x_{t+1} = Ax_t + Bu_t$$

$$y_t = Dx_t + Eu_t$$

$$A = [1.0000]$$

$$B = [7.4307e^{-10}]$$

$$D = [1.4366e^{-5}]$$

$$E = [0.0129]$$

10.5.10. Case Study 2 – mpMPC Model and Tuning Parameters

$$\min_{u} \sum_{k=1}^{OH-1} y_k^T QR_k y_k^T$$

$$s.t.\, x_{k+1} = Ax_k + Bu_k$$

$$y_k = Dx_k + Eu_t$$

$$u_{min} \leq u_k \leq u_{max}$$

$$x_{min} \leq x_k \leq x_{max}$$

$$y_{min} \leq y_k \leq y_{max}$$

Table S12: Case Study 2 - Tuning parameters of the mpMPC controller

Parameter	Value
OH	3
NC	1
QR	10^4
u_{min}	0
u_{max}	4000
x_{min}	-10^9
x_{max}	10^9
y_{min}	0
y_{max}	50